

MassBank

User's Manual

Version 2.4, 7 February 2012

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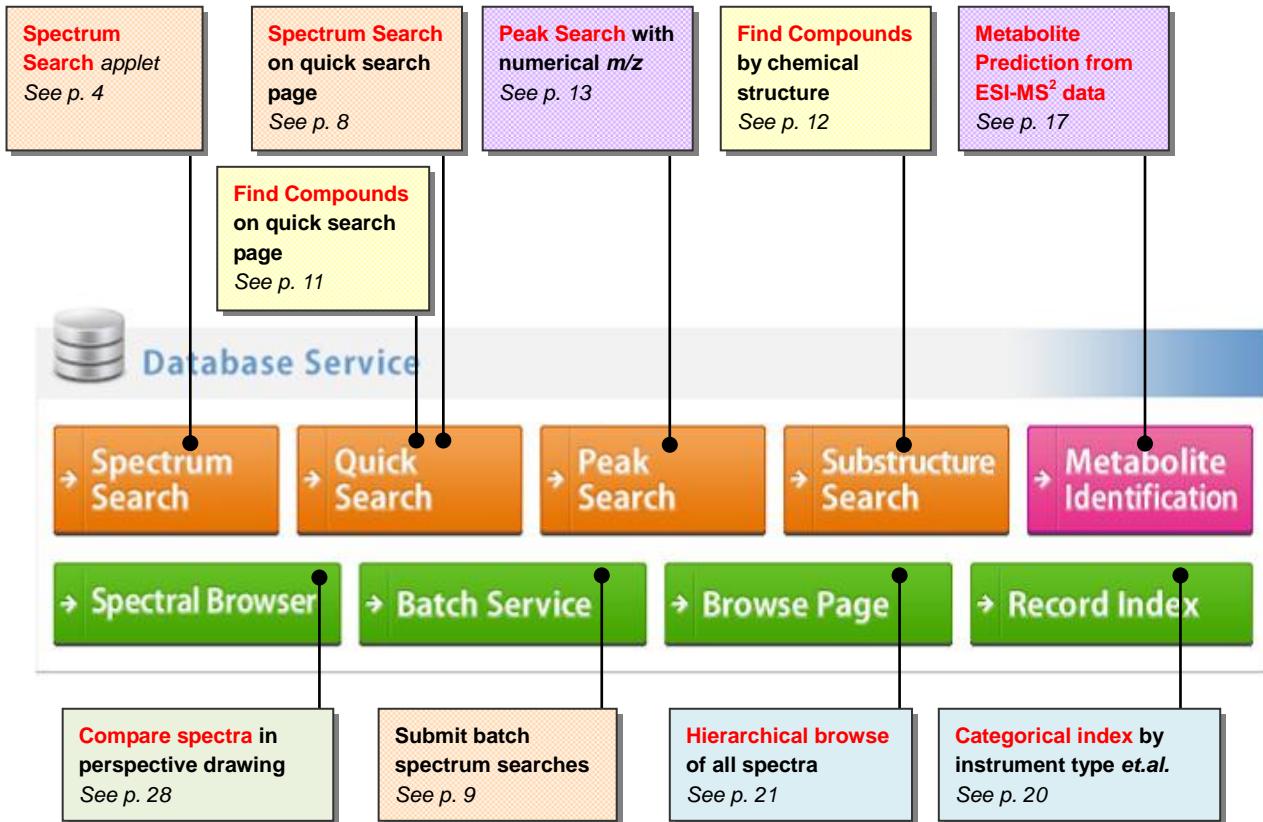
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1. Introduction

This manual mainly describes the operation of the MassBank database services.

1.1 Overview of the Database Services

MassBank provides the following database services.



1.2 System Requirements

Below are the system requirements for using the MassBank database services.

(1) Web Browser

We recommend using Internet Explorer 6 or higher, or Firefox 2 or higher as your browser.

(2) Web Browser Settings

Make sure that your Web browser is configured as follows.

[1] JavaScript execution enabled

[2] Popups enabled

- See the page below for instructions on how to check this (URL to allow: <http://www.massbank.jp>)
http://www.microsoft.com/japan/windowsxp/using/web/sp2_popupblocker.mspx

(3) Install Java runtime environment

The Java Runtime Environment (JRE) Version 5 or higher must be installed.

- You can use the page below to check your installation status and download Java.

<http://www.java.com/en/download/>

2. Searching for Similar Spectra

2.1 Spectrum Search Applet

Spectrum Search enables you to perform GUI-based spectrum searches in a Web browser. Spectra in the MassBank similar to one provided by the user as a query are retrieved and displayed in a list. It is also possible to graphically compare the query spectrum with the retrieved spectrum.

(1) Prepare the query file

When performing a spectrum search with the applet, you must prepare a query file in one of the following formats. A sample can be downloaded from <http://www.massbank.jp/sample/sample.zip>

Name
Write an arbitrary name, such as the name of the compound. (Optional)

Peak information
Write the *m/z* and intensity, separated by spaces. You can write all the peak information on a multiple lines, writing one peak per line.

Empty line
If you include peak information for more than one spectrum, put a blank line between each one.

[Query File Contents]

```

Name: Sample Compound 1
70 24
71 10
72 68
73 999
74 107

Name: Sample_Compound 2
73.1 15008
78.54 4456
79.45 2158311
85.3 964800
86.11 150
90.0 804911

Name: Sample Compound 3
178.876379147 15
186.884786287 8
229.504276894 9

```

Single space
Name : Sample...
 Arbitrary name
 When entering a name, always begin the line with "Name:"

Single space
78.54 4456
m/z Intensity
 (Absolute or relative value can be used)

(2) Load the query and configure the search parameters

Spectrum Search [1]
 After selecting your query file, click **File Read**.

Query list view
 Click **Search Parameter Setting**

After selecting your query file, click **File Read**.

Search Parameter Setting Window

[1] Load the query file

Click **Browse**, and select the query file you have prepared. Click **File Read** to load the file. After the file finishes loading, a list of queries appears.

[2] Set the search parameters

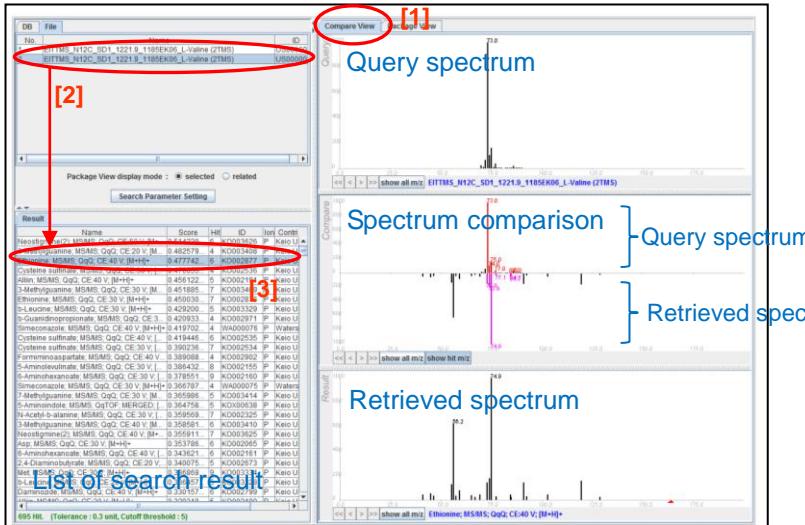
Click **Search Parameter Setting**. The Setting window opens.

Settings

- **Precursor *m/z*** : Precursor ion specified by *m/z*
- **Tolerance** : *m/z* error range
- **Cutoff Threshold** : Relative intensity threshold
- **Instrument Type** : Type of instrument
- **Ionization Mode** : Mode of ionization

(3) Perform the search

Compare View: Compare query and retrieved spectra one to one.



[1] Select "Compare View"

Click to select.

It is selected by default.

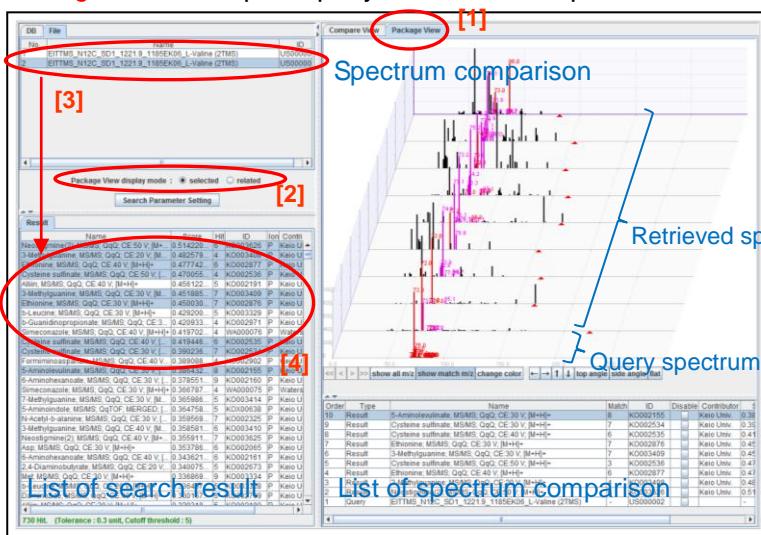
[2] Select the query spectrum

Click to select the spectrum to use in the query. As soon as it is selected, similar spectra are retrieved.

[3] Select a retrieved spectrum

Click to select any spectrum in the list of search result.

Package View: Compare query and retrieved spectra one to many.



[1] Select "Package View"

Click to select.

[2] Select package view display mode

Click "selected" or "related".

[3] Select the query spectrum

Click to select the spectrum to use in the query. As soon as it is selected, similar spectra are retrieved.

[4] Select a retrieved spectrum

Click to select any spectrum in the list of search result. If you chose "selected" in step 2, then you can hold down Ctrl + Shift to select multiple rows. If you chose "related" in step 2, then only one row can be selected.

Different Display Modes in Package View

There are two display modes in Package View.

selected

Multiple spectra can be selected from the list of search results. The selected spectra and the query spectrum are shown in a tiled view.

related

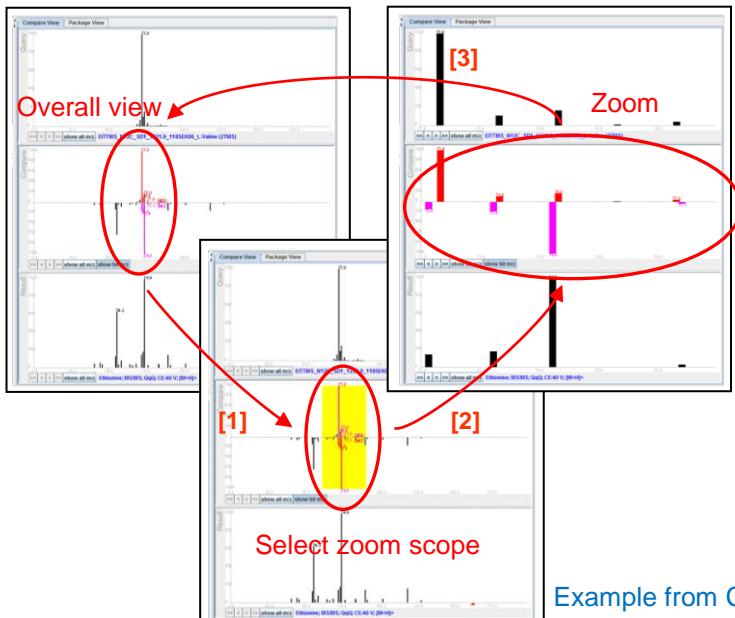
Only one spectrum can be selected from the list of search results. The selected spectrum, a spectrum with different collision energy than the selected spectrum (detected automatically), and the query spectrum are displayed in tiled view.

Peak Color in Spectrum Comparison Window

In the spectrum comparison windows in Compare View and Package View, matching peaks can be distinguished by color.

Peak	Matching m/z on query peak	Perfect Match	Match within Error Margin
Query Spectrum		Red	Red
Retrieved Spectrum		Red	Pink

<<Handy Feature 1: Spectrum Zoom>>

**[1] Select location to zoom**

Drag from the location of the start of the zoom.

[2] Set zoom position

Drop to set the location on the spectrum to zoom.

[3] End zoom

Double click on the spectrum.

Note: You can also zoom on spectrums from the Package View.

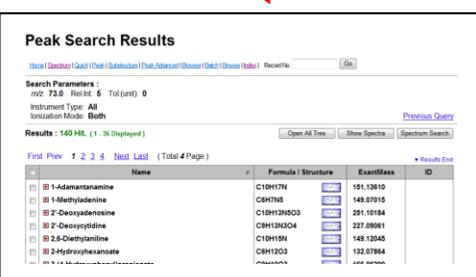
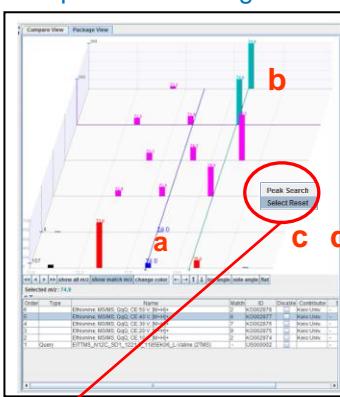
Example from Compare View

<<Handy Feature 2: Peak Manipulation>>

Example from Compare View



Example from Package View



Peak Search Results Window

a. Highlight peak

Place the cursor over a peak. It is highlighted in blue, and the *m/z* and intensity values appear.

b. Select peak

Click on a peak. It is rendered in blue to indicate that it is selected. Up to 6 peaks can be selected.

c. Search for peaks

If you right click while one or more peaks are selected, a menu appears, and "Peak Search" can be selected. The peak search begins immediately after selection.

d. Cancel peak selection

When you right click on the spectrum, a menu appears. Choose "Select Reset".

Peak Rendering Color

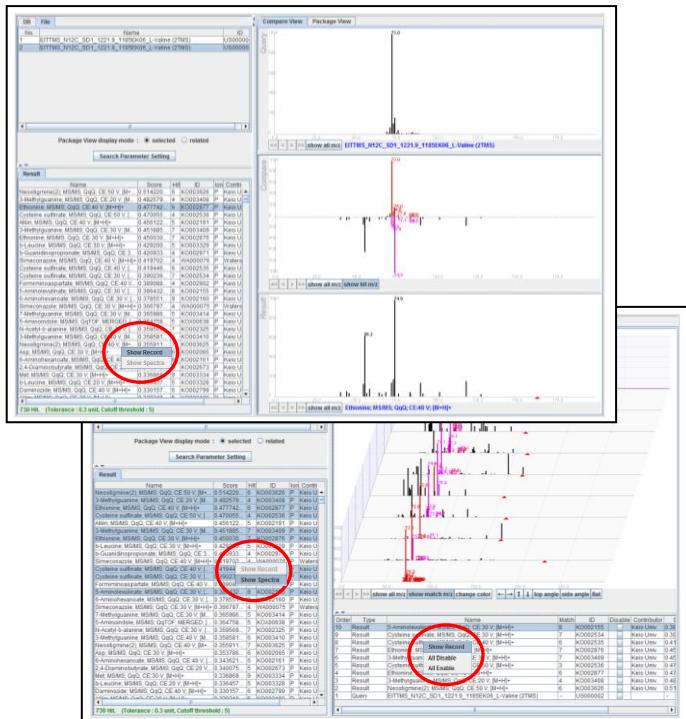
Highlighted: Blue
Selected: Light blue

Highlighting and Selecting Peaks in Package View

When multiple spectrums are displayed in Package View, you can highlight or select the peaks in any spectrum. When you do so, if there is a peak in another spectrum with a perfectly matching *m/z*, then that peak is also highlighted or selected.

<<Handy Feature 3: Show Record>>

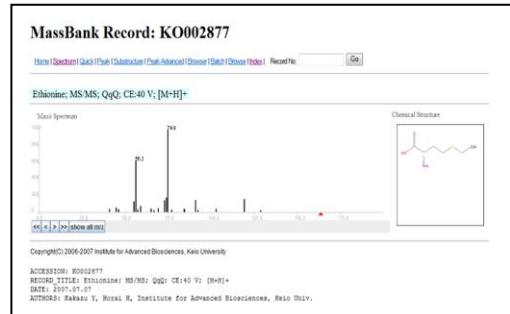
Example from Compare View



Example from Package View

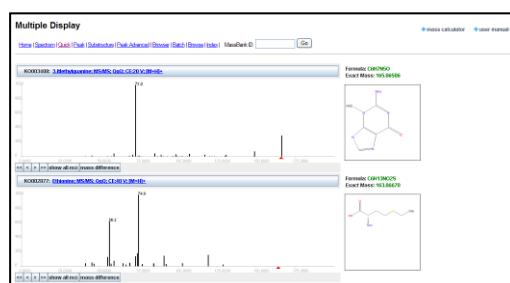
a. Show record

When you right click with one spectrum selected, the "Show Record" command appears on the menu. Select this to view details about the spectrum.



b. Show multiple spectra

When you right click with two or more spectra selected, the "Show Spectra" command appears on the menu. Select this to display multiple spectra in tiled view.



<<Handy Feature 4: Spectrum Manipulation>>



Spectrum Manipulation Buttons in Compare View

<<, <, >, >>
show all m/z
show hit m/z

Move display location (only when zoomed on spectrum)
Display m/z values of all peaks
Display m/z values of matching peaks

Spectrum Manipulation Buttons in Package View

<<, <, >, >>
show all m/z
show match m/z
change color
↔, →, ↑, ↓
top angle
side angle
flat

Move display location (only when zoomed on spectrum)
Display m/z values of all peaks
Display m/z values of matching peaks
Change color of entire spectrum
Change angle (manual manipulation)
Change angle (top perspective)
Change angle (side perspective)
Change angle (all spectra in flat view)

2.2 Spectrum Search on Quick Search Page

The Quick Search feature allows you to search for similar spectra just using simple input.

>> Enter Search Parameters

Quick Search

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | Record No:

[Search by Keyword](#) [Search by Peak](#) Select this

Instrument Type

<input checked="" type="checkbox"/> EI	<input type="checkbox"/> EI-MS
<input checked="" type="checkbox"/> ESI	<input checked="" type="checkbox"/> GC-EI-TOF-MS
<hr/>	
<input checked="" type="checkbox"/> CE-ESI-TOF-MS	
<input checked="" type="checkbox"/> ESI-IT-(MS)n	
<input checked="" type="checkbox"/> ESI-IT-MS/MS	
<input checked="" type="checkbox"/> ESI-QqIT-MS/MS	
<input checked="" type="checkbox"/> ESI-QqQ-MS/MS	
<input checked="" type="checkbox"/> ESI-QqTOF-MS/MS	
<input checked="" type="checkbox"/> LC-ESI-IT-TOF-MS	
<input checked="" type="checkbox"/> LC-ESI-Q-MS	
<input checked="" type="checkbox"/> LC-ESI-TOF-MS/MS	

Ionization Mode

Positive Negative Both

[1] Cutoff threshold of relative intensities [2] Number of Results

Enter peak data

```
273.096 22
289.086 107
290.118 14
291.096 999
292.113 162
293.054 34
579.169 37
580.179 15
```

m/z and relative intensities(0-999), delimited by a space.

[1] Cutoff threshold of relative intensities
 Relative intensity threshold
 Ignore peaks with intensity lower than specified value.

[2] Number of Results
 Number of retrieved spectra to be displayed

Single space
 $273.096 \triangle 22$
 m/z Intensity
 (Absolute or relative value can be used)

>> Display Search Results

Quick Search Results

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | Record No: Go

Query :

Display query spectrum



Results : 20 Hit.

Up to top 20 scores displayed

Hit	Score
8	1.0000
8	0.9054
4	0.6845

Hit: Number of peaks in the retrieved spectra matched to those in a query data

Score: Similarity score of retrieved spectrum to a query data

2.3 Conduct Batch Spectrum Searches

Batch Service conducts a batch spectrum search, and emails you the results.

Use this in such cases as when you would like to search for a large number of spectra.

Batch Service

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#)

This service will appear as a part of Quick Search Page.

[1] Query File: C:\Users\ Desktop\Neg

[2] Mail Address: ttck.keio.ac.jp

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Click **Submit** to perform the batch query. A message appears indicating that the query has been accepted.

Batch Service

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#)

[2009/09/25 18:41:51]
Your batch search is accepted.
The results will be sent to ynihei@ttck.keio.ac.jp later.



Search results are sent to the specified address by e-mail. The following files are attached to the e-mail: (1) Search Results; and (2) Summary of Results.

(1) Search Results (Text Format)

***** MassBank Batch Service Results *****						
Request Date: 2010/10/15 14:07:51 JST						
# Instrument Type: CE-ESI-TOF-MS,ESI-IT-(MS)n,ESI-IT-MS/MS,ESI-QTOF-MS/MS,ESI-QqIT-MS/MS,ESI-QqQ-MS/MS,ESI-QqTOF-MS/MS,LC-ESI-FT-MS,LC-ESI-IT-MS/M S,LC-ESI-IT-TOF-MS,LC-ESI-Q-MS,LC-ESI-QTOF-MS/MS,LC-ESI-QqQ-MS/MS,LC-ESI-TOF-MS						
# Ion Mode: Negative						
# ### Query 1 ###						
# Name: Scan530 Name of a query spectrum						
# Hit: 37						
Top 20 List List of search results (at most 20 high-scored spectra)						
Accession	Title	Formula	Mass	Score	Hit	
KNA00756	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	133.03751	0.3545	2	
KNA00487	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	133.03751	0.3104	2	
KNA00752	L-Serine; LC-ESI-FT-MS; NEG	C3H7NO3	105.04259	0.3041	2	
KNA00542	cis-Aconitate; LC-ESI-FT-MS; NEG	C6H6O6	174.01644	0.2955	2	
KNA00475	L-Serine; LC-ESI-FT-MS; NEG	C3H7NO3	105.04259	0.2942	2	
KNA00628	L-Glutamine; LC-ESI-FT-MS; NEG	C5H10N2O3	146.06914	0.2911	2	
KNA00728	L-Homoserine; LC-ESI-FT-MS; NEG	C4H9NO3	119.05824	0.2904	2	
KNA00812	Citrate; LC-ESI-FT-MS; NEG	C6H8O7	192.027	0.2885	2	
KNA00820	3-Phospho-D-glycerate; LC-ESI-FT-MS; NEG	C3H7O7P	185.99294	0.2844	2	
KNA00554	L-Homoserine; LC-ESI-FT-MS; NEG	C4H9NO3	119.05824	0.2823	2	
KNA00538	sn-Glycerol 3-phosphate; LC-ESI-FT-MS; NEG	C3H9O6P	172.01367	0.2756	2	
KNA00527	(S)-Malate; LC-ESI-FT-MS; NEG	C4H6O5	134.02152	0.2746	2	
KNA00648	L-Threonine; LC-ESI-FT-MS; NEG	C4H9NO3	119.05824	0.2716	2	
KNA00736	L-Asparagine; LC-ESI-FT-MS; NEG	C4H8N2O3	132.05349	0.2713	2	
KNA00808	cis-Aconitate; LC-ESI-FT-MS; NEG	C6H6O6	174.01644	0.2673	2	
KNA00491	L-Glutamine; LC-ESI-FT-MS; NEG	C5H10N2O3	146.06914	0.2663	2	
KNA00483	L-Asparagine; LC-ESI-FT-MS; NEG	C4H8N2O3	132.05349	0.2650	2	
KNA00696	4-Hydroxy-L-proline; LC-ESI-FT-MS; NEGC5H9NO3		131.05824	0.2646	2	
KNA00546	D-Gluconic acid; LC-ESI-FT-MS; NEG	C6H12O7	196.0583	0.2616	2	
KNA00530	2-Oxoglutarate; LC-ESI-FT-MS; NEG	C5H6O5	146.02152	0.2587	2	

(2) Summary of Results (HTMLformat)

Summary Of Batch Service Results

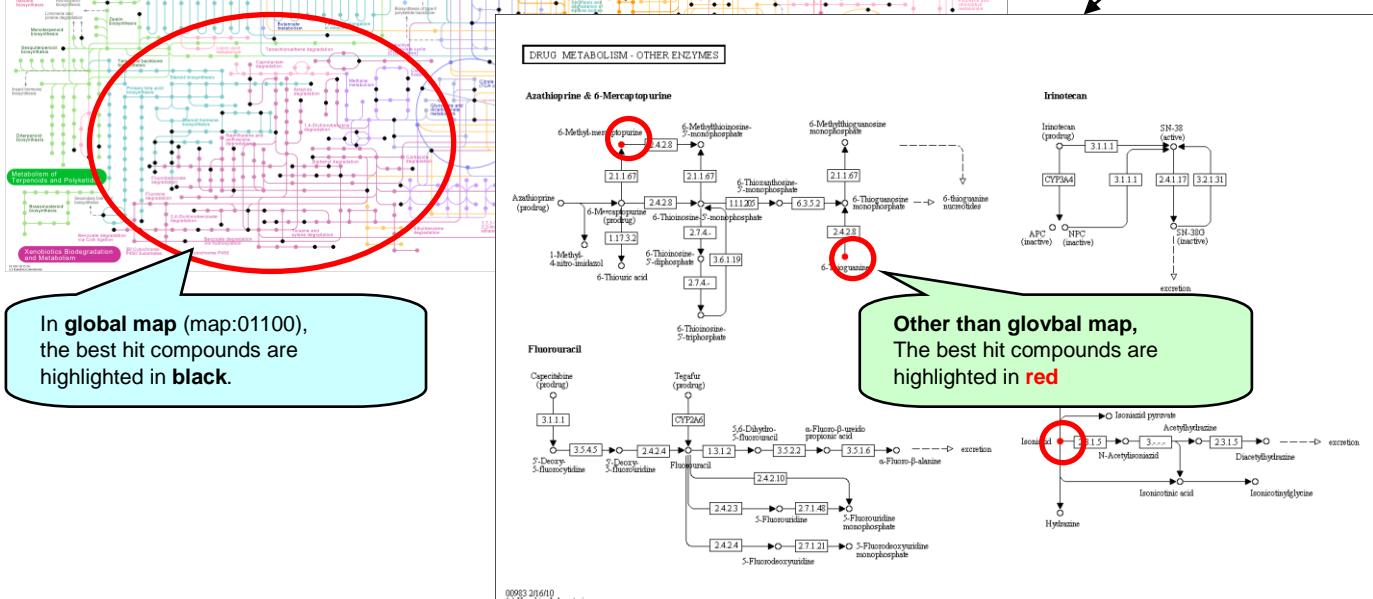
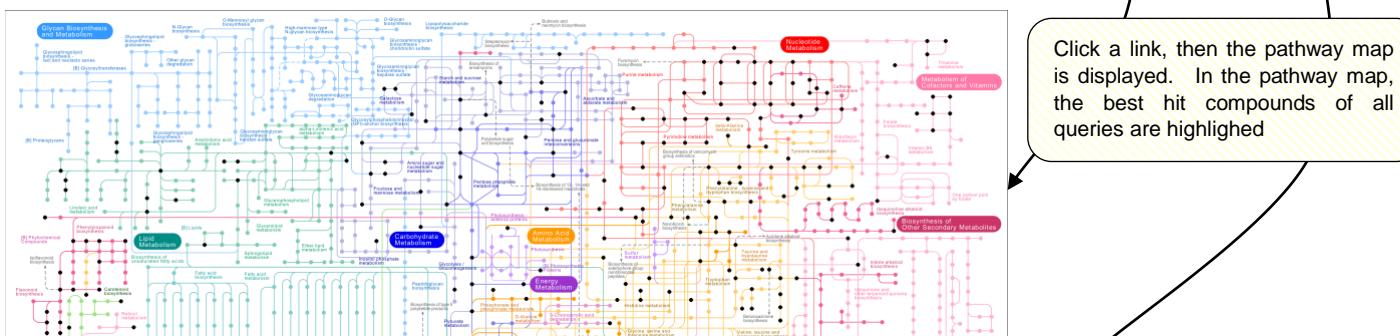
Request Date : 2010/10/15 14:07:51 JST

Instrument Type : CE-ESI-TOF-MS, ESI-IT-(MS), ESI-IT-MS/MS, ESI-QTOF-MS/MS, ESI-QqQ-IT-MS/MS, ESI-QqQ-MS/MS, ESI-QqTOF-MS/MS, LC-ESI-FT-MS, LC-ESI-IT-MS/MS, LC-ESI-IT-TOF-MS, LC-ESI-O-MS, LC-ESI-QTOF-MS/MS, LC-ESI-Qq-MS/MS, LC-ESI-TOF-MS

Ion Mode : Negative

List of the best hit for each query

No.	Query Name	Score	MassBank ID	Record Title	Formula	KEGG ID	Colored Pathway Maps			
							MAP1	MAP2	MAP3	MAP4
1	Scan530	0.3545	KNA00756	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	C00049	map:01100(28)	-	-	-
2	Scan531	0.9999	K0001625	Propionate; MS/MS; QqQ; CE10 V; [M-H]-	C3H2O2	C00804	-	-	map:00640(1)	-
3	Scan532	0.2593	KNA00475	L-Serine; LC-ESI-FT-MS; NEG	C3H7NO3	C00065	map:01100(28)	-	-	-
4	Scan534	0.3524	KNA00756	L-Aspartate; LC-ESI-FT-MS; NEG	C4H7NO4	C00049	map:01100(28)	-	-	-
5	Scan535	0.9899	K0001625	Propionate; MS/MS; QqQ; CE10 V; [M-H]-	C3H2O2	C00804	-	-	map:00640(1)	-
6	Scan538	No Hit Record								
7	Scan539	0.0751	UT002896	Phosphatidylethanolamine alkanyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84N07P	-	-	-	-	-
8	Scan540	0.4198	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
9	Scan542	No Hit Record								
10	Scan543	0.1230	UT002896	Phosphatidylethanolamine alkanyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84N07P	-	-	-	-	-
11	Scan544	0.4294	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
12	Scan546	0.0876	UT00244	Phosphatidylserine 18:1-22:0 / 20:0-20:1; LC-MS/MS; Orbitrap; m/z: 844.61; [M-H]-; RT: 51.49; Exp: 2	C47H80N09P	-	-	-	-	-
13	Scan547	0.5831	PR050557	Acetylsalicylic acid; ESI-QTOF-MS/MS; MERGED; [M-H]-	C9H8O4	-	-	-	-	-
14	Scan548	0.1290	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
15	Scan550	0.3157	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
16	Scan551	0.4388	WA000541	Pentobarbital sodium salt; LC-Q/MS; NEG; 30 V	C11H17N2NaO3	-	-	-	-	-
17	Scan552	0.1185	TY000116	Baicalein; LC-ESI-IT-MS/MS; [M-H]-	C21H18O11	-	-	-	-	-
18	Scan554	0.2840	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
19	Scan555	0.1109	UT002896	Phosphatidylethanolamine alkanyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84N07P	-	-	-	-	-
20	Scan556	0.5934	PR050557	Acetylsalicylic acid; ESI-QTOF-MS/MS; MERGED; [M-H]-	C9H8O4	-	-	-	-	-
21	Scan558	No Hit Record								
22	Scan559	0.1074	UT002896	Phosphatidylethanolamine alkanyl 18:0-24:5; LC-MS/MS; Orbitrap; m/z: 804.59; [M-H]-; RT: 37.85; Exp: 3	C47H84N07P	-	-	-	-	-
23	Scan560	0.1286	PB004142	Kaempferol; MS/MS; QqQ; CE35 eV; [M-H]-	C15H10O6	C05903	map:01100(28)	-	-	-
24	Scan562	No Hit Record								
25	Scan563	0.2191	UT002452	Phosphatidylserine 18:0-20:1 / 18:1-20:0; LC-MS/MS; Orbitrap; m/z: 816.57/729.15; [M-H]-/[M-Ser]-; RT: 43.92; Exp: 2	C45H86N09P	-	-	-	-	-
26	Scan564	0.4068	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	-
27	Scan566	No Hit Record								
28	Scan567	0.0201	MT000095	taurochenodeoxycholate; MS/MS; IT; m/z: 498.3; [M-H]-	C26H45NO6S	C05485	-	-	-	map:0121(1)
29	Scan568	0.4064	TY000102	Cinobufotalin; LC-ESI-IT-TOF-MS; [(M+CH3COOH)-H]-	C26H34O7	-	-	-	-	map:0121(1)



3. Compound Search

3.1 Find Compounds on Quick Search Page

The Quick Search feature allows you to search for compounds by compound name, molecular formula, etc.

>> Enter Search Parameters

Quick Search

Select this : | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | Record No: []

 manual (in Japanese)

Search by Keyword Search by Peak

[1] Compound Name acetate

AND [2] Exact Mass [] Tolerance 0.3

AND [3] Formula []
(e.g. C6H7N5, C5H*N5, C5*)

Reset

Search

You can narrow your results by selecting the Instrument type and Ionization Mode.

Instrument Type

- | | | |
|--|---|--|
| <input checked="" type="checkbox"/> EI | <input type="checkbox"/> EI-MS | <input checked="" type="checkbox"/> GC-EI-TOF-MS |
| <input type="checkbox"/> ESI | <input type="checkbox"/> CE-ESI-TOF-MS | <input type="checkbox"/> ESI-IT-(MS)n |
| | <input type="checkbox"/> ESI-IT-MS/MS | <input type="checkbox"/> ESI-QqT-MS/MS |
| | <input type="checkbox"/> ESI-QqQ-MS/MS | <input type="checkbox"/> ESI-QqTOF-MS/MS |
| | <input type="checkbox"/> LC-ESI-IT-TOF-MS | <input type="checkbox"/> LC-ESI-Q-MS |
| | <input type="checkbox"/> LC-ESI-TOF-MS/MS | |

Ionization Mode

- Positive Negative Both

[1] Compound Name

Enter the compound name. Names with substring matches on the string you entered are retrieved.

[2] Exact Mass/Tolerance

Enter the exact mass and error tolerance.

[3] Formula

Enter the molecular formula of the compound. Enter the formula starting with "C", followed by "H", and then the other letters in alphabetical order. Add wildcards ("*") to find partial matches.

Example: C5H*N5

>> Display Search Results



Quick Search Results

 mass calculator  user manual

Search Parameters :

Compound Name acetate

Instrument Type: GC-EI-TOF-MS

Ionization Mode: Positive

[Edit / Resubmit Query](#)

Results : 4 Hit. (1 - 4 Displayed)

Matching items (including synonyms) are displayed

Search

First Prev 1 Next Last (Total 1 Page)

▼ Results End

Name	Formula / Structure	ExactMass	ID
3,4-dihydroxyphenylacetic acid	C8H8O4 	168.04226	
4-Hydroxyphenylacetic acid	C8H8O3 1 spectrum 	152.04734	
Indole-3-acetic acid	C10H9NO2 2 spectra 	175.06333	

First Prev 1 Next Last (Total 1 Page)

▲ Results Top

3.2 Find Compounds by Chemical Structure

The Substructure Search enables you to find compounds including the specified chemical structure.

>> Enter Search Parameters

Substructure

Query1

Query2

AND

[1] [2]

Edit Molfile Clear

Query2

Edit Molfile Clear

(1) Number of π electrons

Comparison of pi-electron for each atom. **number in query = number in target**

* Double and triple bound is translated to pi-electrons of the bonded atoms.

Copyright 2008 by K. Tanaka and S. Kanaya, NAIST, Japan.

Peak Search (Option)

m/z , ,
Tolerance of m/z 0.3

Search **(2) Peak Search option**

(1) Number of π electrons

- Query structure = target structure (default)
- Query structure \leq target structure
- No comparison

(2) Peak Search option

Specify m/z values to perform peak search at same time.

You can also narrow your results by selecting the Instrument type or Ionization Mode.



>> Display Search Results

Query1

Query structure

Edit / Resubmit Query

Results : 48 Hit. (1 - 42 Displayed)

Open All Tree Multiple Display Spectrum Search

First Prev 1 2 Next Last (Total 2 Page)

▼ Results End

	Name	Formula / Structure	ExactMass	ID
<input type="checkbox"/>	(R)-(-)-Phenylephrine	C9H13NO2	167.09463	
<input type="checkbox"/>	1,10-Phenanthroline	C12H8N2	180.06875	

Enter query structure

[1] Write in editor

JME Molecular Editor®, Novartis Pharma AG

OK CANCEL JME Editor courtesy of Peter Ertl, Novartis

Or:

[2] Load Molfile

Read Molfile

参照...

OK CANCEL

(1) Click Browse

ファイルのアップロード フォルダ

名前 更新日時 種類 サイズ

KO000001.mol KO000012.mol KO000023.mol KO000034.
KO000002.mol KO000013.mol KO000024.mol KO000035.
KO000003.mol KO000014.mol KO000025.mol KO000036.
KO000004.mol KO000015.mol KO000026.mol KO000037.
KO000005.mol KO000016.mol KO000027.mol KO000038.
KO000006.mol KO000017.mol KO000028.mol KO000039.
KO000007.mol KO000018.mol KO000029.mol KO000040.
KO000008.mol KO000019.mol KO000030.mol KO000041.
KO000009.mol KO000020.mol KO000031.mol KO000042.
KO000010.mol KO000021.mol KO000032.mol KO000043.
KO000011.mol KO000022.mol KO000033.mol KO000044.

ファイル名(N): KO00002.mol

すべてのファイル 開(O) キャンセル

(2) Select a file

The loaded structure formula can be modified in the editor as well.

4. Peak Search

4.1 Peak Search by *m/z* values

Peak Search enables you to find peaks by specifying the *m/z* or *m/z* difference as numerical values.

>> Enter Search Parameters

- [1] Search of Peaks Peak Differences
 [2] Search by m/z-Value Molecular Formula

[3] m/z	[4] Formula
AND <input type="button" value="m/z"/>	C6H7
AND <input type="button" value="m/z"/>	<input type="button" value="C6H7"/>
AND <input type="button" value="m/z"/>	<input type="button" value="C6H7"/>
AND <input type="button" value="m/z"/>	<input type="button" value="C6H7"/>
AND <input type="button" value="m/z"/>	<input type="button" value="C6H7"/>
AND <input type="button" value="m/z"/>	<input type="button" value="C6H7"/>
Rel.Intensity 100	Tolerance 0.3
<input type="button" value="Search"/> <input type="button" value="Reset"/>	

[1] Search of "Peaks" or "Peak Differences"

- "Peaks": search of the *m/z* value.
- "Peak Differences": search of the *m/z* differences.

[2] Search by "m/z-Value" or "Molecular Formula"

Select "m/z-Value" for Peak Search by *m/z* values.

[3] *m/z*

Specify the peak *m/z* value. You can specify up to 6, and connect them via AND or OR conditions.

[4] Rel. Intensity

Ignore peaks with intensity lower than specified value. Specify a relative intensity from 1 to 999.

[5] Tolerance

Specify the *m/z* error range.

Converting from molecular formula to *m/z*

Enter a molecular formula the exact calculated mass in the *m/z* text box. The exact calculated mass is truncated to 5 decimal place.

You can also narrow your results by selecting the Instrument type or Ionization Mode.

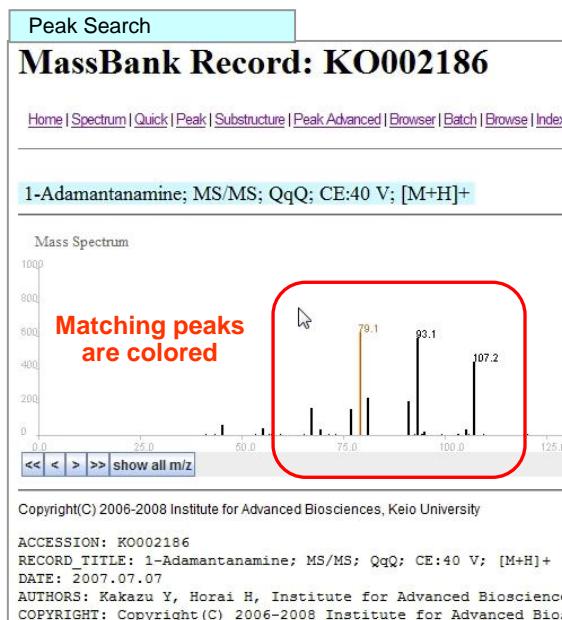
>> Display Search Results

Results : 313 Hit. (1 - 46 Displayed)

First Prev 1 2 3 4 5 6 7 8 9 Next Last (Total 9 Page)

	Name	Formula / Structure	ExactMass
<input type="checkbox"/>	1-Adamantanamine	C10H17N	151.13610
<input type="checkbox"/>	MS/MS; QqQ; CE:40 V; [M+H]+	C10H17N	151.13610
<input type="checkbox"/>	MS/MS; QqQ; CE:50 V; [M+H]+	C10H17N	151.13610
<input type="checkbox"/>	MS/MS; QqTOF; MERGED; [M+H]+	C10H17N	151.13610
<input type="checkbox"/>	1-Methyladenine	C6H7N5	149.07015
<input type="checkbox"/>	MS/MS; QqQ; CE:40 V; [M+H]+	C6H7N5	149.07015
<input type="checkbox"/>	MS/MS; QqQ; CE:50 V; [M+H]+	C6H7N5	149.07015

>> Spectrum View



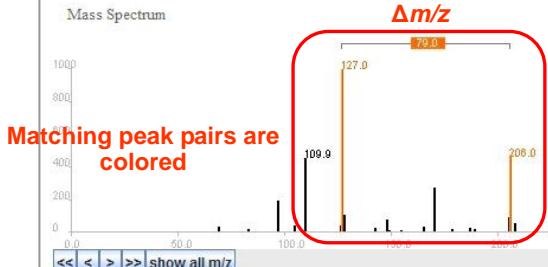
Peak Difference Search

MassBank Record: KO002304

Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse

5-Aminoimidazole-4-carboxamide-1-ribofuranosyl 5'-monopho

Mass Spectrum



4.2 Peak Search with Molecular Formulas

Peak Search Advanced enables you to find peaks by specifying an ion or neutral loss by molecular formulas instead of a numerical m/z values.

>> Enter Search Parameters

Searching via ion

Search of Peaks Peak Differences
 Search by m/z-Value Molecular Formula

Ion 1	Ion 2	Ion 3	Ion 4
Formula	Formula	Formula	Formula
<input type="text" value="C5H6N5"/>	<input type="text" value="C3H6N"/>	<input type="text"/>	<input type="text"/>
AND	AND	AND	AND
<input checked="" type="radio"/> AND	<input type="radio"/> OR	Enter molecular formula	

Search

If CH₃COOH is entered, it is converted internally to C₂H₄O₂ for the search.

>> Display Search Results

Query:

Ion 1 C5H6N5 AND **Ion 2** C3H6N

Edit / Resubmit Query

Results : 1 Hit. (1 - 1 Displayed)

First Prev **1** Next Last (Total **1** Page)

The screenshot shows a software interface for metabolite identification. A list of metabolites is displayed, with the first item, "S-Adenosylmethionine", being the focus. This item's name is circled in red and has a blue arrow pointing from it to a yellow callout box containing the text "Click link". To the right of the metabolite list, there is a small icon representing a spectrum and the text "1 spectrum". At the top right of the interface, the text "C15H2" is visible.

>> Spectrum View

Searching by Ion

MassBank Record: KOX00710 MERGED SPECTRUM

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | Record No.:

Dihydrophosphingosine; MS/MS; QqTOF; MERGED; [M+H]⁺

Mass Spectrum

C18H40NO₂

Molecular formulas with matching peaks appear

m/z	Relative Abundance
254.289	~100
302.308	~1000
326.8611	~100

<< < > >> show all m/z

Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University

ACCESSION: KOX00710
 RECORD TITLE: Dihydrophosphingosine; MS/MS; QqTOF; MERGED; [M+H]⁺

Searching via neutral loss

Search of Peaks Peak Differences
 Search by m/z-Value Molecular Formula

Neutral Loss 1	Neutral Loss 2	Neutral Loss 3	Neutral Loss 4
Formula C4H7NO2	Formula CH4S	Formula	Formula

AND SEQUENCE

Enter molecular formula

* The targets of Peak Search Advanced are only Keio and Riken data.

[Search](#) |

If "SEQUENCE" is selected, peak pairs, whose m/z difference is matched to the molecular formula, are retrieved in the order of Neutral Loss 1, 2, and 3. (In the example above, order of CH₄H₇NO₂, then CH₄S)

Query :

Neutral Loss 1	Neutral Loss 2
C4H7NO2	CH4S

[Edit / Resubmit Query](#)

Results : 1 Hit. (1 - 1 Displayed)

First Prev **1** Next Last (Total **1** Page)

MS/MS: QqTOF: MERGED: [M+H]+

Click link

Searching by Neutral Loss

MassBank Record: KOX00636 MERGED SPECTRUM

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | [Record No.](#)

S-Adenosylmethionine; MS/MS; QqTOF; MERGED; [M+H]⁺

Mass Spec

CH₄S

CH₄S

C₄H₇NO₂

1000
800
600
400
200
0

0.0 100.0 200.0 300.0 400.0

02.057

240.005

298.165

399.152

<< < > >> show all m/z

Molecular formulas with matching peak pairs

* Assist in the Input of Molecular Formulas

When *m/z* values instead of molecular formulas are entered in the "Formula" boxes, a list of candidate molecular formulas, whose exact masses are close to the entered *m/z* values, is shown in the pull-down menu.

Following example shows a case when a value, 141, was entered in a Formula box on the "Search of Peaks" and "Search by Molecular Formula" mode.

<p>Search of <input checked="" type="radio"/> Peaks <input type="radio"/> Peak Differences</p> <p>Search by <input type="radio"/> <i>m/z</i>-Value <input checked="" type="radio"/> Molecular Formula</p> <table border="1" style="width: 100%; border-collapse: collapse; font-family: monospace;"> <tr> <th style="width: 33%;">Ion 1</th> <th style="width: 33%;">Ion 2</th> <th style="width: 33%;">Ion 3</th> </tr> <tr> <td>Formula</td> <td>Formula</td> <td>Formula</td> </tr> <tr> <td>141 </td> <td>AND</td> <td>AND</td> </tr> <tr> <td colspan="3"> C6H5O2S (141.00103) X C7H6ClO (141.01072) C6H5O4 (141.01878) C9H5N2 (141.04527) C6H9N2O2 (141.0664) C11H9 (141.07043) C6H13N4 (141.11402) See C9H17O (141.12794) C8H17N2 (141.13917) </td> </tr> </table> <p>Copyright © since 2006-2010 JST-BIRD MassBank</p>	Ion 1	Ion 2	Ion 3	Formula	Formula	Formula	141	AND	AND	C6H5O2S (141.00103) X C7H6ClO (141.01072) C6H5O4 (141.01878) C9H5N2 (141.04527) C6H9N2O2 (141.0664) C11H9 (141.07043) C6H13N4 (141.11402) See C9H17O (141.12794) C8H17N2 (141.13917)			<p>Search of <input checked="" type="radio"/> Peaks <input type="radio"/> Peak Differences</p> <p>Search by <input type="radio"/> <i>m/z</i>-Value <input checked="" type="radio"/> Molecular Formula</p> <table border="1" style="width: 100%; border-collapse: collapse; font-family: monospace;"> <tr> <th style="width: 33%;">Ion 1</th> <th style="width: 33%;">Ion 2</th> <th style="width: 33%;">Ion 3</th> </tr> <tr> <td>Formula</td> <td>Formula</td> <td>Formula</td> </tr> <tr> <td style="border: 2px solid red;">C6H5O4</td> <td>AND</td> <td>AND</td> </tr> <tr> <td colspan="3"> <input checked="" type="radio"/> AND <input type="radio"/> OR </td> </tr> </table> <p>* The targets of Peak Search Advanced are only Keio and Riken data</p> <p style="text-align: center;">Search</p> <p>Copyright © since 2006-2010 JST-BIRD MassBank</p>	Ion 1	Ion 2	Ion 3	Formula	Formula	Formula	C6H5O4	AND	AND	<input checked="" type="radio"/> AND <input type="radio"/> OR		
Ion 1	Ion 2	Ion 3																							
Formula	Formula	Formula																							
141	AND	AND																							
C6H5O2S (141.00103) X C7H6ClO (141.01072) C6H5O4 (141.01878) C9H5N2 (141.04527) C6H9N2O2 (141.0664) C11H9 (141.07043) C6H13N4 (141.11402) See C9H17O (141.12794) C8H17N2 (141.13917)																									
Ion 1	Ion 2	Ion 3																							
Formula	Formula	Formula																							
C6H5O4	AND	AND																							
<input checked="" type="radio"/> AND <input type="radio"/> OR																									

Pull-down menu shows a list of the molecular formulas, whose exact masses is starting from the value 141. No molecular formula such as 140.9 are listed because prefix string match algorithm is applied.

5. Prediction of Metabolites from ESI-MS² Data

5.1 Metabolite prediction by using peak-chemical substructure relationships

Currently this tool is adapted to predict primary metabolites and their derivatives from the query ESI-MS² data. MassBank has analyzed and accumulated the relationships between peaks (product ions) and chemical substructures by chemically annotating ESI-MS² data of primary metabolites.

The present tool elucidates possible chemical substructures of the unknown metabolite from the query ESI-MS² data by using the relationships that linked the observed product ions to chemical substructures. Additionally possible molecular formulae of the unknown metabolite are predicted from the precursor ion. KNApSAcK database < http://kanaya.naist.jp/knapsack_isp/top.html > provides a list of metabolites that satisfy the predicted molecular formula with the possible chemical substructures. Finally the prediction tool outputs the list as the candidates of the unknown metabolite.

A reliable prediction is expected when (1) the query ESI-MS² data should be analyzed on high resolution mass analyzers, (2) the precursor ion observed is a type of "M + H", (3) more than ten product ions with the relative intensity higher than 5 % are observed, (4) a query data that was prepared by merging two or more ESI-MS² data analyzed on the same unknown metabolite at different CID conditions gives a good result. The present tool automatically merges them into a single query data.

>> Input the query data and set the parameters

The following procedure shows a case when three ESI-MS² data analyzed on the same unknown metabolite at different CID conditions are uploaded, merged into a single query data, and predicted.

Metabolite Identification

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Identification](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID: Go

[1]

by Peak-Substructure Relationships

by Annotated Neutral Losses

[2]

Query File

sample file sample archive



A list of the ESI-MS² data uploaded is shown.

[1] Select "by Peak-Substructure Relationships"

[2] Load the query file*

- Select the query file.
- Click "File Read".

*To prepare the query ESI-MS² file, see "2.1 (1) Prepare the query file".

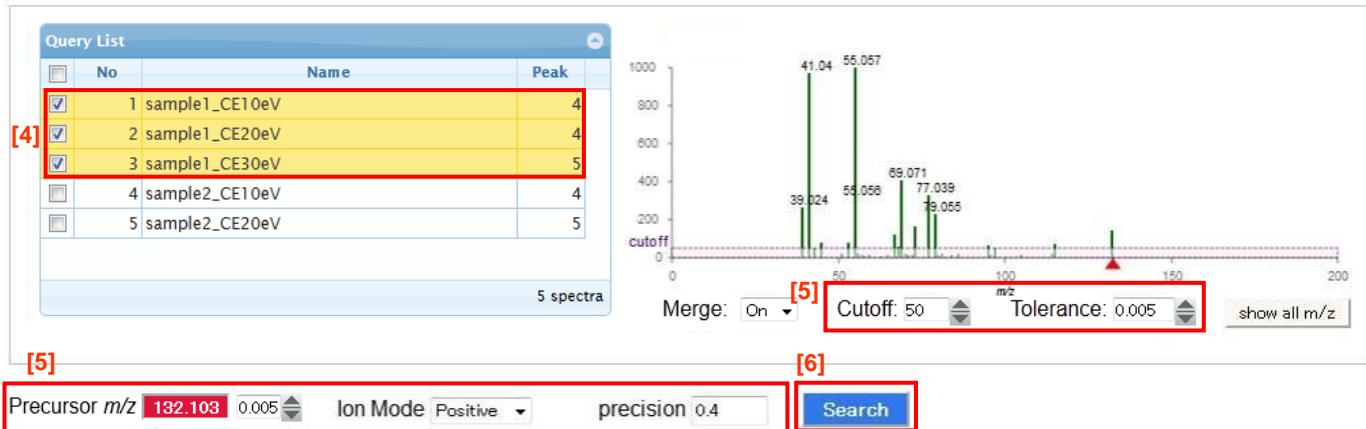


Precursor m/z Ion Mode precision

[3] Set "Merge On"

- A check box [3'] is appeared at each data.





[4] By checking the box, select the data files of the metabolite to be identified.

- As one data is selected by checking the box, it is added and merged into the query.
- With each selection, the merged ESI-MS² data generated is shown in the right window

[5] Set parameters (see the table below)

- All the parameters should be set correctly.
- Input "Precursor m/z".

I61 Click "Search" button to start.

– Parameters settings –

• Merge:

Select "ON" when two or more ESI-MS2 data are merged into the query. Check box is appeared at each data. Select the data by checking their boxes.
Leave "OFF" (default) to predict the metabolite from a single data.

• Cutoff:

This selects the product ions for the prediction.
Only the peaks larger than the cutoff value are considered in the prediction.
Cutoff value is indicated by the red dotted line on the merged spectra in the write window.
Precursor ion is always included in the prediction independent of the cutoff value.

• Tolerance:

This defines the mass accuracy of the product ions in the query data. Within the tolerance, substructure-peak relationships give possible substructures to each product ion.

• Precursor m/z in the red box:

Check whether the precursor m/z is correct.
When the m/z value is not correct, correct it manually.

• Precursor m/z in the white box:

This defines the mass accuracy of the precursor m/z.

• Ion Mode:

Select either "Positive" or "Negative".

• Precision:

This is the precision of an empirical relationship between a peak and a chemical substructure that is used for prediction. False positive decreases with the precision. See the next page for details.

>> Search Results

Matched Formulae : 4

m/z	78.0355	80.0508	96.0458	123.0560
Formula	C5H4N	C5H6N	C5H6NO	C6H7N2O
No.	ion-pos-0013	ion-pos-0013	ion-pos-0013	ion-pos-0013

Hit Relationships : 2

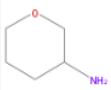
ion-pos-0013 Substructure



Formula, Precision & Recall, TP

C5H4N	0.66	0.68	27
C6H7N2O	0.67	0.1	4
C5H6N	0.71	0.38	15
Others	0.00	0.00	0

ion-pos-0028 Substructure



Formula, Precision & Recall, TP

C5H6NO	0.55	0.55	11
Others	0.00	0.00	0

A

- **m/z:** Product ions used for prediction
- **Formula:** Possible molecular formulae assigned to the ions
- **No:** ID numbers of the substructures predicted by the relationships between peaks and chemical substructures

* By placing the cursor on an ID number, the corresponding substructure is shown as "A".

Results : 3 Hit.

Isonicotineamide

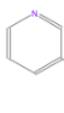


Formula : C6H6N2O
Exact Mass : 122.048

DB Links
KEGG : [C02421](#)

Hit Relationship-No.
ion-pos-0013

Nicotinamide

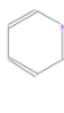


Formula : C6H6N2O
Exact Mass : 122.04801

DB Links
KNAPSAck : [C00000209](#)
KEGG : [C00153](#)

Hit Relationship-No.
ion-pos-0013

Picolinamide



Formula : C6H6N2O
Exact Mass : 122.048

DB Links
KEGG : [C01950](#)

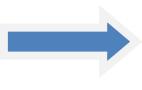
Hit Relationship-No.
ion-pos-0013

B

A: Possible substructures that are embedded in the structure of the unknown metabolite are predicted by using the relationships between peaks and chemical substructures.

B: Candidates of the unknown metabolite are shown. The KNAPSAck database outputs the candidates that satisfy the following conditions; they have one or more of the substructures shown in A and the molecular formula is the same to that predicted from the mass of the precursor ion. A substructure in the gray box in A is not applicable in the candidates in B.

Formula, Precision & Recall, TP			
C5H4N	0.66	0.68	27



C5H4 \longleftrightarrow precision 0.66
recall 0.68



Formula, Precision & Recall, TP: ("C5H4N", "0.66", "0.68", "27" in the above example)

Formula: Chemical formula of a peak

Precision: Ratio of the number of ESI-MS² data (pyrimidine substructure & C5H4N) to that of ESI-MS² data (C5H4N), where among the ESI-MS² data (C5H4N), in which the peak C5H4N was observed, ESI-MS² data (pyrimidine substructure & C5H4N) are those analyzed on chemical compounds with the pyrimidine substructure. In the above example, the ratio is 0.66.

Recall: Ratio of the number of ESI-MS² data (pyrimidine substructure & C5H4N) to that of ESI-MS² data (pyrimidine substructure), where the ESI-MS² data (pyrimidine substructure) were analyzed on chemical compounds with the pyrimidine substructure. In the above example, the ratio is 0.68.

TP: Total number of the ESI-MS² data (pyrimidine substructure & C5H4N). In the above example, it is 27.

5.2 Metabolite prediction by spectrum search in terms of neutral loss

Chemical compounds are often synthesized from a common chemical compound by slight chemical modifications. Such derivatives share the chemical structure of the common chemical compound. Their mass spectra are also similar, although their similarity cannot be detected by conventional spectral similarity search. Peaks observed in the mass spectrum of one derivative are shifted by $\Delta m/z$ from the corresponding peaks of the other one where $\Delta m/z$ is the mass difference between their chemical structures. Such a similarity is searchable by comparing not the m/z of the corresponding peaks but the mass difference between the corresponding peak pairs because $\Delta m/z$ is unknown. Thus this tool searches the ESI-MS² data in MassBank that are similar to the query one by comparing the m/z difference between the corresponding peak pairs. Here “neutral loss” is defined as the m/z difference between peak pairs. Search results suggest the users the common chemical compound among the target and query chemical compounds. However, this comparison has such a general difficulty that many possible peak pairs should be compared within the mass accuracy of m/z . To escape the difficulty, the targets in the present method are limited to the high resolution MassBank ESI-MS² data with chemical annotation on peaks. All possible peak differences in each target data have been calculated not by m/z but by the assigned molecular formulae. MassBank recommends the query data that is enough high in the resolution to assign the molecular formula to peaks. All possible peak differences in the target are also calculated by the molecular formulae. Peak differences between the target and the query are compared by the molecular formulae. Additionally the present tool evaluates the matching peaks observed in the range of m/z 50-99.

>> Input the query data and set the parameters

Metabolite Identification

[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Identification](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID: Go

by Peak-Substructure Relationships by Annotated Neutral Losses [1]

 Query File

 参照...

 File Read

 sample file  sample archive

Search similar spectra on a neutral loss-to-neutral loss basis

Retrieves spectra similar to user's spectrum in terms of molecular formulae.

This search is helpful to predict the chemical structure of unknown metabolites.

[1] Select “by Annotated Neutral Losses”.

[2] - [6] the same in the Section 5.1 “Metabolite prediction based on peak-chemical substructure relationships”.

>> Search Results

Matched neutral losses : 6
H3N(17.027), CH2N2(42.022), C4H6(54.047), CH5N3(59.048), C3H7O(59.05), C4H9N(71.074)

Results : In descending order of number of matched neutral loss.

No. 1 PR100307 Agmatine; LC-ESI-QTOF-MS/MS; CE:Ram, 5-6 ... <p>Neutral Loss Hits : 5 H3N(17.027) CH2N2(42.022) C4H6(54.047) CH5N3(59.048) C4H9N(71.074)</p> <p>Ion CH6N3(60.05617) C4H10N(72.08132)</p> <p>Formula : C5H14N4 Exact Mass : 130.12185</p>	No. 2 KOX00653 Agmatine; MS/MS; QqTOF; MERGED; [M+H]+ <p>Neutral Loss Hits : 5 H3N(17.027) CH2N2(42.022) C4H6(54.047) CH5N3(59.048) C4H9N(71.074)</p> <p>Ion CH6N3(60.05617) C4H10N(72.08132)</p> <p>Formula : C5H14N4 Exact Mass : 130.12185</p>	No. 3 KOX00672 Buformin; MS/MS; QqTOF; MERGED; [M+H]+ <p>Neutral Loss Hits : 4 H3N(17.027) CH2N2(42.022) CH5N3(59.048) C4H9N(71.074)</p> <p>Ion CH6N3(60.05617) C4H10N(72.08132)</p> <p>Formula : C6H15N5 Exact Mass : 157.13275</p>
No. 4 KOX00641 N-Acetylputrescine; MS/MS; QqTOF; MERGED ... <p>Neutral Loss Hits : 3 H3N(17.027) C4H6(54.047) C4H9N(71.074)</p> <p>Ion C4H10N(72.08132)</p> <p>Formula : C6H14N2O Exact Mass : 130.11061</p>	No. 5 KOX00781 Metformin; MS/MS; QqTOF; MERGED; [M+H]+ <p>Neutral Loss Hits : 3 H3N(17.027) CH2N2(42.022) CH5N3(59.048)</p> <p>Ion CH6N3(60.05617)</p> <p>Formula : C4H11N5 Exact Mass : 129.10145</p>	No. 6 KOX00737 <i>b</i> -Guanidinopropionate; MS/MS; QqTOF; MERGED ... <p>Neutral Loss Hits : 3 H3N(17.027) CH2N2(42.022) CH5N3(59.048)</p> <p>Ion CH6N3(60.05617) C4H10N(72.08132)</p> <p>Formula : C4H9N3O2 Exact Mass : 131.06948</p>

A list of the peak differences that were annotated with the molecular formula in the query data.

* MassBank data similar to the query one are shown (max. 30 data).

(1) Neutral Loss: Here “Neutral Loss” is defined as the difference of the corresponding peak pairs in terms of molecular formulae. The target data are listed by a total number (**Hits**) of the molecular formulae that were matched between the query and target ESI-MS² data.

(2) Ion: The matching peaks ($50 < m/z < 99$) are listed by molecular formulae.

- A. They are shown in a dotted red box when the target data have the maximum number of matching peaks.
- B. The target data that have no matching peak are shown in a grey box. They are not shown when the “**hide**” button was clicked.
- C. “Results: **NO peaks within m/z 50-99 in query.**” is shown when no peak ($50 < m/z < 99$) was observed in the query data.
- D. “Results: **NO matched ions to peaks within m/z 50-99 in query.**” is shown when no peak ($50 < m/z < 99$) has no annotated molecular formulae.

(3) Exact Mass: Molecular mass of the target data is shown in white characters in the red box or in the grey box when it is equal to “Precursor $m/z +1$ ” or “Precursor $m/z -1$ ” in the positive or negative mode, respectively.

(4) Rank: The target data are listed by the rank which is scored by a total number of matching peak pairs with matching peaks.

Minimum requirements that target data are matched or similar to the query are as follows.

- Target data are ranked at high.
- They have one or more matching peaks ($50 < m/z < 99$).
- Their molecular mass is equal to that of the query.

6. Browsing All Data

6.1 Categorical Index

In Record Index, all data is categorized into contributor, instrument type, MS type, merged type, ion mode and compound name categories. Click a link in this page, then the whole data in the category is displayed in the same format as other search results.

Record Index

⊕ mass calculator ⊕ user manual

Home | Spectrum | Quick | Peak | Substructure | Advanced | Browser | Batch | Browse | Index | MassBank ID: Go

Contributor	: Chubu Univ. (2,628) IMM, CAMS & PUMC, China (67) Kyoto Univ. (185) NAIST (817) Osaka Univ. (502) Tottori Univ. (16) Univ. Toyama (253)	Fac. Eng. Univ. Tokyo (12,379) Kazusa (273) LeibnizIPB (528) Nihon Univ. (75) PFOS research group (277) UOEH (35) Waters (2,994)	Fukuyama Univ. (340) Keio Univ. (5,629) Metabolon (149) Osaka MCHRI (20) RIKEN (1,722) Univ. Connecticut (510)		
Instrument Type	: CE-ESI-TOF (20) EI-EBEB (12) ESI-QqQ-MS/MS (52) FAB-EB (5) FI-B (1) LC-ESI-IT (515) LC-ESI-Q (2,721) LC-ESI-QTOF (2,742)	CI-B (796) ESI-IT-MS/MS (149) ESI-QqTOF-MS/MS (510) FAB-EBEB (173) GC-EI-TOF (1,016) LC-ESI-ITFT (3,006) LC-ESI-QIT (378) MALDI-TOF (17)	EI-B (11,636) ESI-QqIT-MS/MS (15) FAB-B (26) FD-B (41) LC-APPI-QQ (277) LC-ESI-ITTOF (253) LC-ESI-QQ (5,038)		
MS Type	: MS (16,898)	MS2 (11,505)	MS3 (926)	MS4 (70)	
Merged Type	: Normal (28,560)	Merged (839)			
Ion Mode	: Positive (22,721)	Negative (6,678)			
Compound Name	: A (1,273) G (747) M (1,552) S (948) Y (8)	B (1,117) H (565) L (1,389) I (1,491) Z (75)	C (1,478) I (777) Q (471) U (118) J (3) P (3,762) V (137) Others (623)	D (1,887) L (3) P (3,762) W (3) E (760) K (216) Q (140) X (50)	E (395) L (1,371) B (262) X (50)

[1] Contributor

Number of data listed by contributors.

Each link is followed by the parenthesized number of spectra in the category.

[2] Instrument Type

Number of data listed by the types of chromatography and mass spectrometer.

[3] MS Type

Number of data listed by the types of mass spectrometry.

[4] Merged Type

Number of merged ESI-MS2 data and that of the other data.

[5] Ionization Mode

Number of data analyzed by positive and negative modes.

[6] Compound Name

Number of data listed by the first letters of compound names.

6.2 Hierarchical Browse

In Browse Page, all data are hierarchically displayed for each data provider. You can go up and down the hierarchy (tree) and find a specific data you want.

Browse Page

mass calculator user manual (in Japanese)

Home | Spectrum | Quick | Peak | Substructure | Peak Advanced | Browser | Batch | Browse | Index | MassBank ID: _____ Go

[1] [2] [3]

After selecting a spectrum by clicking , you can select multiple spectra by clicking  with Ctrl key or Shift key.

After that, a right button click shows the following popup menu.

[case of single selection]

Show Record
Multiple Display

Click "Show Record", then the details of the MassBank Record are displayed.

[case of multiple selection]

Show Record
Multiple Display

Click "Multiple Display", then multiple spectra are displayed in tiled view.

[1] Select Provider

Click a radio button, then display the hierarchy of the selected provider is displayed in right hand side.

[2] Browse Tree

 : open the lower layer.
 : close the lower layer.

[3] Display Spectrum

View detailed MassBank Record: Double click of ; or "Show Record" in popup menu by right button click when a spectrum is selected.

Display multiple spectra in a tiled view: "Mutiple Display" in popup menu by right button click when multiple spectra are selected.

7. Others

7.1 Search Results

When you conduct a search via "Quick Search", "Substructure Search", "Peak Search", "Peak Search Advanced", or "Record Index", the search results are displayed in a common format.

<<Operation 1>>

List of Search Results

Compound list

Results : 25 Hit. (1 - 25 Displayed)			
First Prev 1 Next Last (Total 1 Page)			
Name	Formula / Structure	ExactMass	ID
2,4-Dimethylaniline	C8H11N	121.08915	
2,6-Diethylaniline	C10H15N		
2,6-Dimethylaniline	C8H11N	121.08915	

Click the "+" icon to expand an individual tree.

Open All Tree Multiple Display Spectrum Search ▾ Results End			
Name	Formula / Structure	ExactMass	ID
2,4-Dimethylaniline	C8H11N	121.08915	
2,6-Diethylaniline	C10H15N		
2,6-Dimethylaniline	C8H11N	121.08915	

Expand all trees

Click on a column heading to sort (by name, molecular formula, or exact mass).

Spectrum list

Results : 25 Hit. (1 - 25 Displayed)			
First Prev 1 Next Last (Total 1 Page)			
Name	Formula / Structure	ExactMass	ID
2,4-Dimethylaniline	C8H11N	121.08915	KO002806
2,6-Diethylaniline	C10H15N	149.12045	KO002677
2,6-Dimethylaniline	C8H11N	121.08915	KO002801

Click link

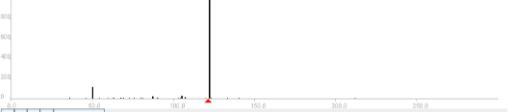
Close All Tree Multiple Display Spectrum Search ▾ Results End			
Name	Formula / Structure	ExactMass	ID
2,4-Dimethylaniline	C8H11N	121.08915	KO002806
2,6-Diethylaniline	C10H15N	149.12045	KO002677
2,6-Dimethylaniline	C8H11N	121.08915	KO002801

MassBank Record: KO002806

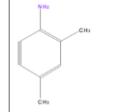
[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Peak Advanced](#) | [Browse Batch](#) | [Browse Index](#) | Record No. Go

2,4-Dimethylaniline; MS/MS; QqQ; CE:10 V; [M+H]⁺

Mass Spectrum



Chemical Structure



Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University.

ACCESSION: KO002806
RECORD NO.: 2,4-Dimethylaniline; MS/MS; QqQ; CE:10 V; [M+H]⁺
DATE: 2007-07-10
AUTHORS: Kakazu Y, Morai M, Institute for Advanced Biosciences, Keio Univ.
COPYRIGHT: Copyright(C) 2006-2008 Institute for Advanced Biosciences, Keio University

MassBank record of an individual spectral data is displayed.

<<Operation 2>>

Interaction with "Multiple Display" and "Spectrum Search"

Results : 25 Hit. (1 - 25 Displayed)

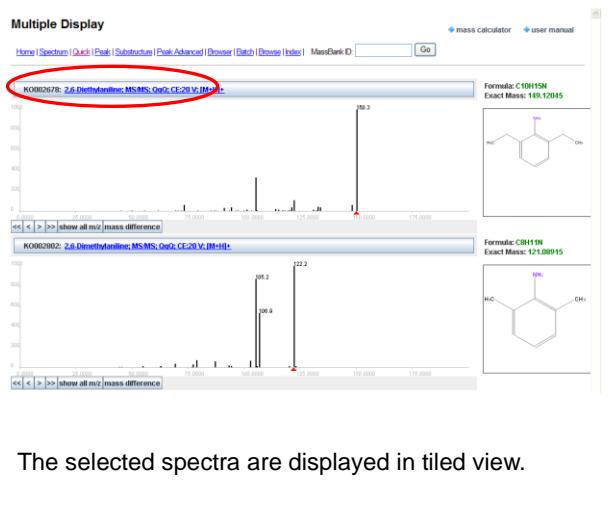
Close All Tree Multiple Display Spectrum Search

First Prev 1 Next Last (Total 1 Page)

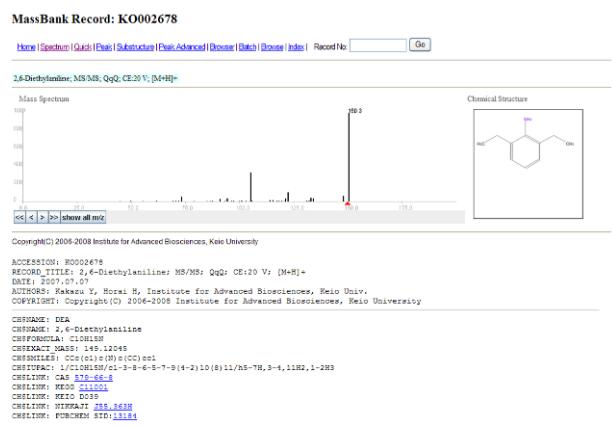
	Name	Formula / Structure	
<input type="checkbox"/>	2,4-Dimethylaniline	C8H11N 	5 spectra K0002806 K0002807 K0002808 K0002809 K0002810
<input type="checkbox"/>	2,6-Diethylaniline	C10H15N 	5 spectra 149.12045 MS/MS: QqQ, CE:10 V; [M+H]+ MS/MS: QqQ, CE:20 V; [M+H]+ MS/MS: QqQ, CE:30 V; [M+H]+ MS/MS: QqQ, CE:40 V; [M+H]+ MS/MS: QqQ, CE:50 V; [M+H]+
<input checked="" type="checkbox"/>	2,6-Diethylaniline	C8H11N 	5 spectra 121.08915 MS/MS: QqQ, CE:10 V; [M+H]+ MS/MS: QqQ, CE:20 V; [M+H]+ MS/MS: QqQ, CE:30 V; [M+H]+ MS/MS: QqQ, CE:40 V; [M+H]+ MS/MS: QqQ, CE:50 V; [M+H]+

[1] Select checkbox to select spectrum
[2] Click either of the buttons

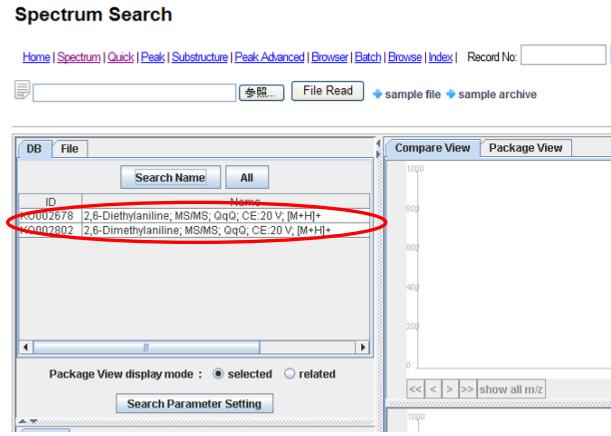
Clicking "Show Spectra"



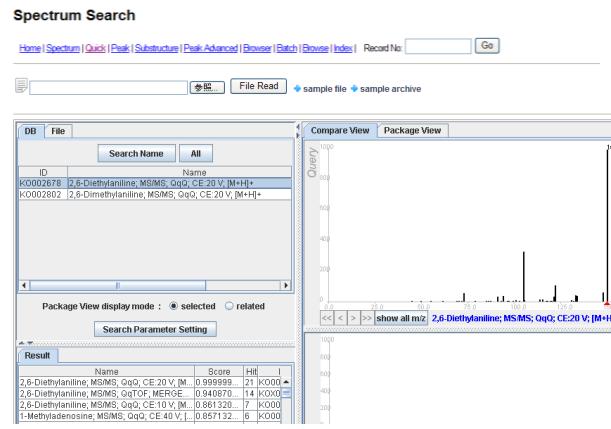
Click a button displaying a record title to show the MassBank record.



Clicking "Spectrum Search"



You can search with the selected spectrum as the query.



<<Operation 3>>

Brief display of chemical structure

Results : 5,704 Hit. (1 - 182 Displayed) Open All Tree Multiple Display Spectrum Search

First Prev [1](#) [2](#) [3](#) [4](#) [5](#) [6](#) [7](#) [8](#) [9](#) [10](#) Next Last (Total 28 Page) ▾ Results End

	Name	Formula / Structure	ExactMass	ID
<input type="checkbox"/>	(9Z, 12Z)-Octadecadienoate	C18H32O2 6 spectra	280.24023	
<input type="checkbox"/>	(Aminomethyl)phosphonate	CH6NO3P 12 spectra		
<input type="checkbox"/>	(Methylthio)acetate	C3H6O2S 6 spectra		
<input type="checkbox"/>	(R)-Mandelate	C8H8O3 5 spectra	152.04734	
<input type="checkbox"/>	(S)-2-Aminobutyrate	C5H10NO2 11 spectra	103.06333	

1) Move mouse pointer onto a thumbnail of chemical structure

2) The structure is enlarged.
If mouse pointer leaves from the thumb nail, then it disappears

(9Z, 12Z)-Octadec...

Results : 5,704 Hit. (1 - 182 Displayed) Open All Tree Multiple Display Spectrum Search

Total 28 Page) ▾ Results End

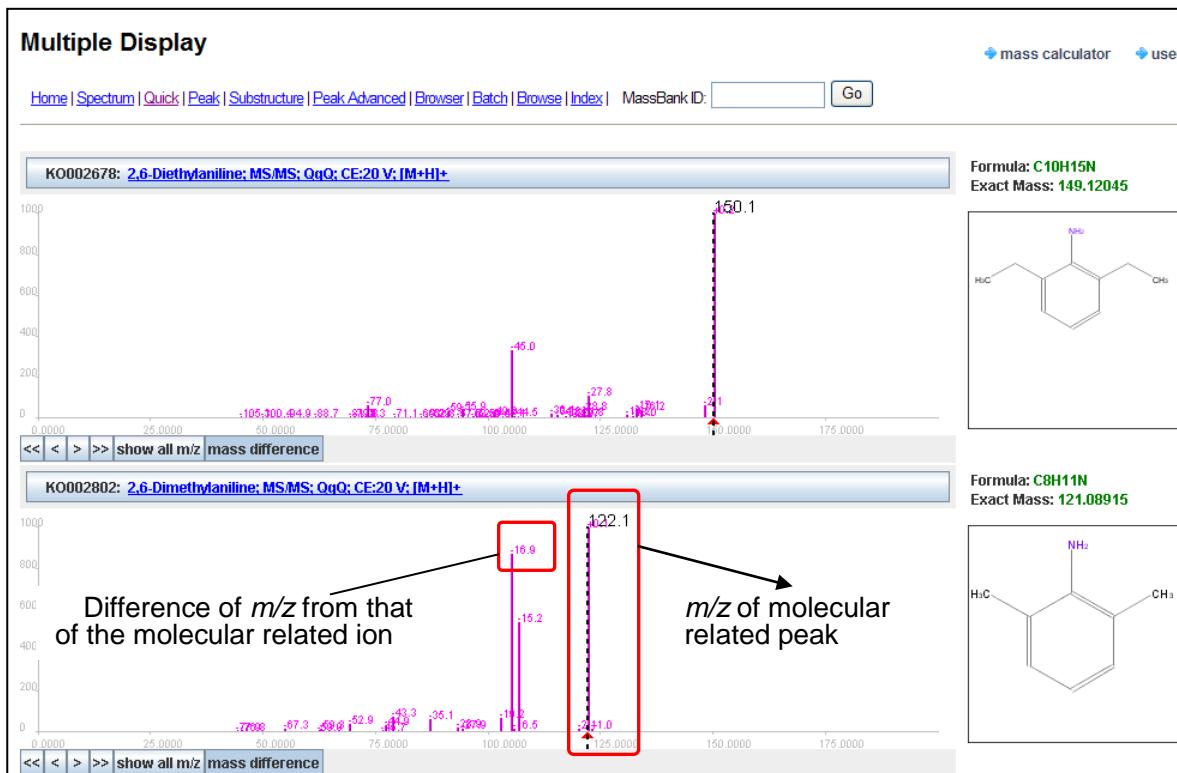
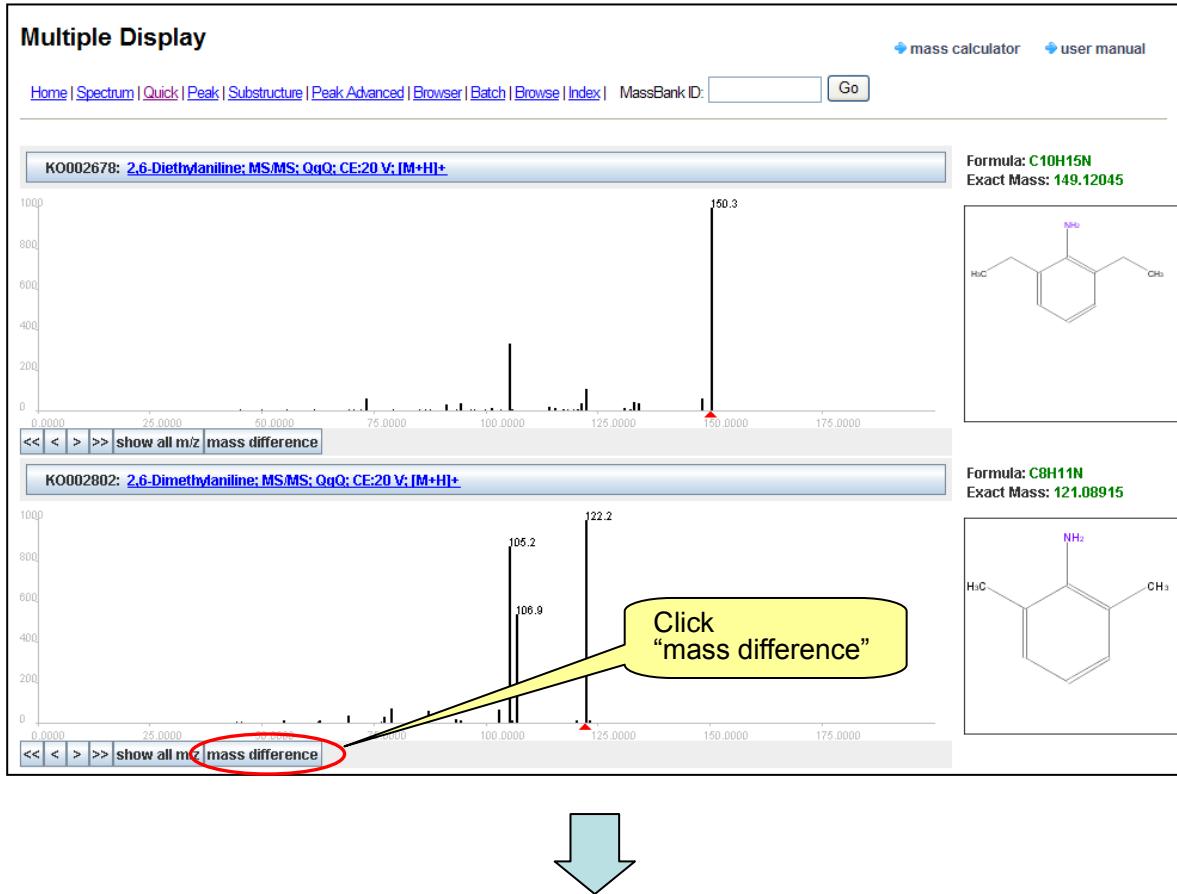
	Formula / Structure	ExactMass	ID
<input type="checkbox"/>	C18H32O2 6 spectra	280.24023	
<input type="checkbox"/>	CH6NO3P 12 spectra		
<input type="checkbox"/>	C3H6O2S 6 spectra		
<input type="checkbox"/>	C8H8O3 5 spectra	152.04734	
<input type="checkbox"/>	(S)-2-Aminobutyrate 11 spectra	103.06333	

1) Click a thumbnail of chemical structure.

2) Large strcuture is shown in another window.
If another thumbnail is clicked, then a new window does not appear and the new structure is shown in the window.
It does not disappear automatically, then you must close the window by yourself

>> mass difference

When click the "mass difference" button on the "Multiple Display" panel of "Compound and Peak Search Results", spectra display the peaks with the value of m/z difference from that of the molecular related ion.



7.2 MassBank Record Detailed Display

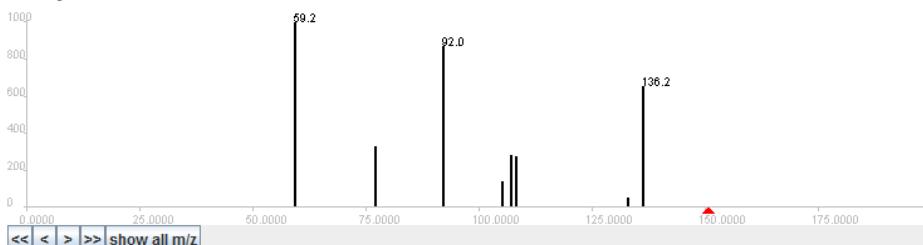
The MassBank record is the fundamental unit of data in the MassBank database. Each mass spectrum has one MassBank record. In addition to peak data, each record includes the compound information (CH\$), test conditions (AC\$), etc. (To see "Record Editor Manual" for more details)

MassBank Record: K0001419

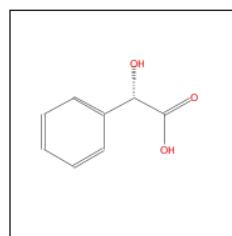
[Home](#) | [Spectrum](#) | [Quick](#) | [Peak](#) | [Substructure](#) | [Identification](#) | [Browser](#) | [Batch](#) | [Browse](#) | [Index](#) | MassBank ID: Go

(S)-Mandelic acid; LC-ESI-QQ; MS2; CE:30 V; [M-H]-

Mass Spectrum



Chemical Structure



ACCESSION: K0001419
 RECORD_TITLE: (S)-Mandelic acid; LC-ESI-QQ; MS2; CE:30 V; [M-H]-
 DATE: 2011.05.10 (Created 2007.07.07)
 AUTHORS: Kakazu Y, Horai H, Institute for Advanced Biosciences, Keio
 LICENSE: CC BY-NC-SA
 COMMENT: KEIO_ID M057

CH\$NAME: (S)-Mandelate
 CH\$NAME: (S)-Mandelic acid
 CH\$NAME: (S)-2-Hydroxy-2-phenylacetic acid
 CH\$NAME: (S)-2-Hydroxy-2-phenylacetate
 CH\$COMPOUND_CLASS: Non-Natural Product
 CH\$FORMULA: C8H8O3
 CH\$EXACT_MASS: 152.04734
 CH\$SMILES: OC(=O)[C@H](O)C(C)CCCC
 CH\$IUPAC: InChI=1S/C8H8O3/c9-7(8(10)11)6-4-2-1-3-5-6/h1-5,7,9H,(H,10
 CH\$LINK: CAS [90-64-2](#) [611-72-3](#)
 CH\$LINK: CHEBI [32800](#)
 CH\$LINK: CHEMPDB [SMN](#)
 CH\$LINK: KEGG [C01984](#)
 CH\$LINK: PUBCHEM SID:[5081](#)

AC\$INSTRUMENT: API3000, Applied Biosystems
 AC\$INSTRUMENT_TYPE: LC-ESI-QQ
 AC\$MASS_SPECTROMETRY: MS_TYPE MS2
 AC\$MASS_SPECTROMETRY: ION_MODE NEGATIVE
 AC\$MASS_SPECTROMETRY: COLLISION_ENERGY 30 V

MS\$FOCUSSED_ION: PRECURSOR_M/Z 151
 MS\$FOCUSSED_ION: PRECURSOR_TYPE [M-H]-

PK\$NUM_PEAK: 8
 PK\$PEAK: m/z int. rel.int.
 59.200 707921.5 999
 77.200 232673.5 328
 92.000 613862.0 866
 105.100 99010.0 140
 107.200 198020.0 279
 108.300 193069.5 272
 133.000 34653.5 49
 136.200 460396.5 650

//

Base Info

ACCESSION: "record ID"
 RECORD_TITLE: "title (compound name, method, etc.)"
 DATE: "Date last updated (Create date)"
 AUTHORS: "Record creators"
 LICENSE: "Creative Commons or Copyright"

Compound Info

CH\$NAME: "name (can include multiple names, including variants)"
 CH\$FORMULA: "Molecular formula"
 CH\$EXACT_MASS: "Exact mass (to five decimal places)"
 CH\$SMILES: "SMILES code"
 CH\$IUPAC: "InChI code"

Analytical Conditions

AC\$INSTRUMENT: "instrument name"
 AC\$INSTRUMENT_TYPE: "instrument type"
 AC\$MASS_SPECTROMETRY: MS_TYPE "ms type"
 AC\$MASS_SPECTROMETRY: ION_MODE "ion mode"

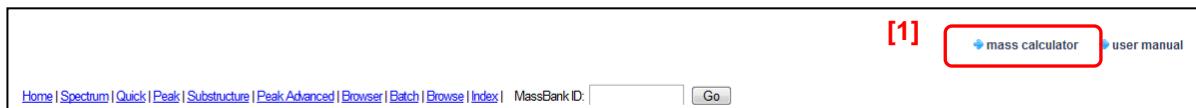
Peak Data

PK\$NUM_PEAK: number of peaks
 PK\$PEAK: array of m/z, measured intensity, and relative intensity for each peak

* For details of MassBank Record, see "Record Editor Manual".

7.3 Basic Mass Calculation Tool

Mass Calculator on the upper right corner is a basic mass calculation tool that you can use everywhere in MassBank. It calculates m/z (i.e. exact mass) of the input formula or displays a list of chemical formulae corresponding to m/z .

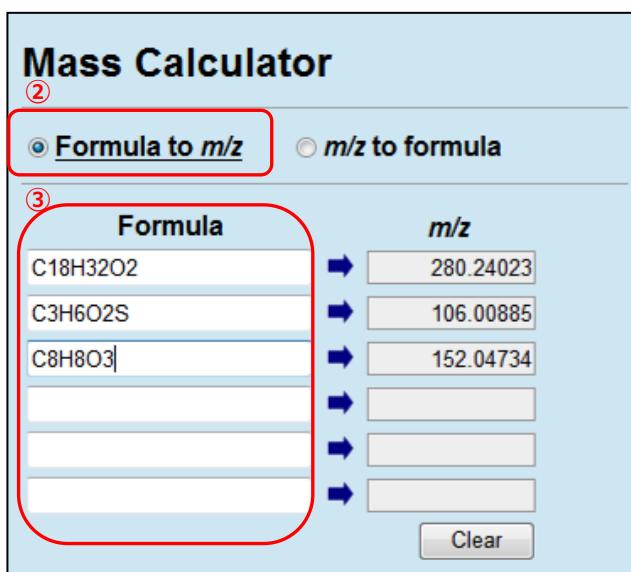


[1] Click "mass calculator"

MassCalculator appears in a separate window.



Calculation of m/z from chemical formula.



Formula	m/z
C18H32O2	280.24023
C3H6O2S	106.00885
C8H8O3	152.04734

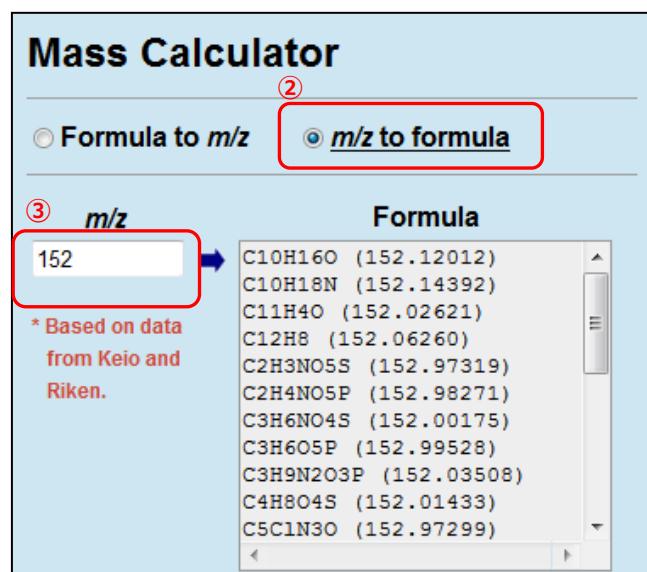
Clear

[1] Select "Formula to m/z "

[3] Input Formula

When a formula is entered, m/z is calculated and displayed.

Listing of chemical formulae corresponding to m/z .



m/z	Formula
152	C10H16O (152.12012)
	C10H18N (152.14392)
	C11H4O (152.02621)
	C12H8 (152.06260)
	C2H3NO5S (152.97319)
	C2H4NO5P (152.98271)
	C3H6NO4S (152.00175)
	C3H6O5P (152.99528)
	C3H9N2O3P (152.03508)
	C4H8O4S (152.01433)
	C5C1N3O (152.97299)

* Based on data from Keio and Riken.

[2] Select " m/z to formula"

[3] Input m/z

When a m/z value is entered, the chemical formulae that were observed in the MassBank annotated ESI-QTOF-MS² data are shown.

Chemical formulae listed are those that were actually observed in Keio and RIKEN ESI-QTOF-MS² data, but not possible chemical formulae.

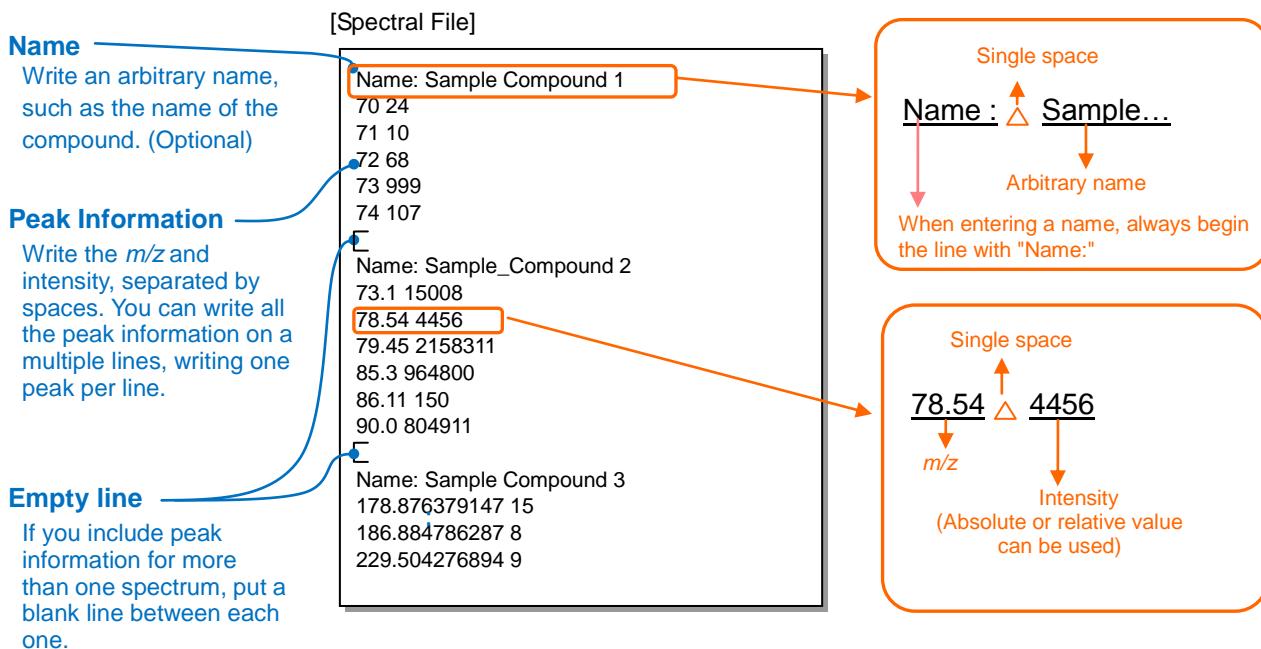
Mass Calculator window can be closed by ESC key.

7.4 Comparison Tool of User Spectra

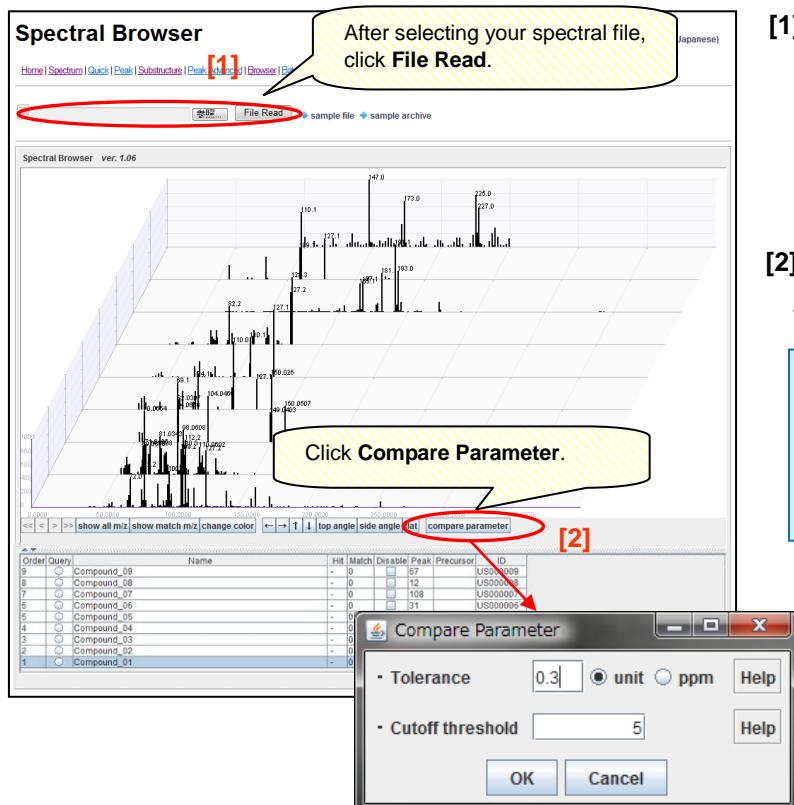
Spectral Browser is a comparison tool of spectra which reads a file which consists of a set of user spectra and displays them in perspective drawing. The upper limit of user spectra is 20. It also compare input spectra each other.

(1) Prepare the spectral file

The format of an input of Spectral Brower, so-called a spectral file, is as follows. You can download a sample from <http://www.massbank.jp/sample/sample.zip>. The format of this spectral file is same as the format of a query file of Spectrum Search, then a spectral file is commonly used in Spectrum Search, Spectral Brower.



(2) Load spectral file and set the compare parameters



[1] Load the spectral file

Click "Browse", and select a spectral file. Afterwards, click "File Read", then Spectral Brower reads the spectral file and display the spectra in it

[2] Set the compare parameters

Click Compare Parameter.
The Setting window opens.

Settings

- Tolerance:** m/z error range
- Cutoff Threshold:** Relative intensity threshold

Compare Parameter Setting Window

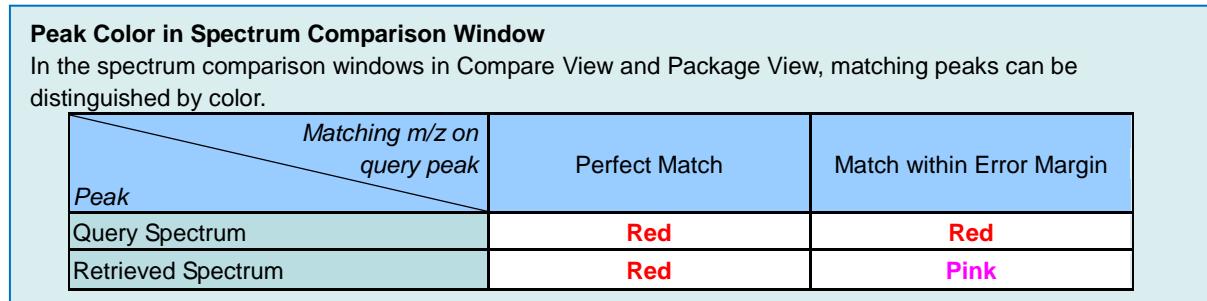
(3) Perform the compare

When you specify an arbitrary spectrum as a query, then you can compare input spectra in one-to-many manner.

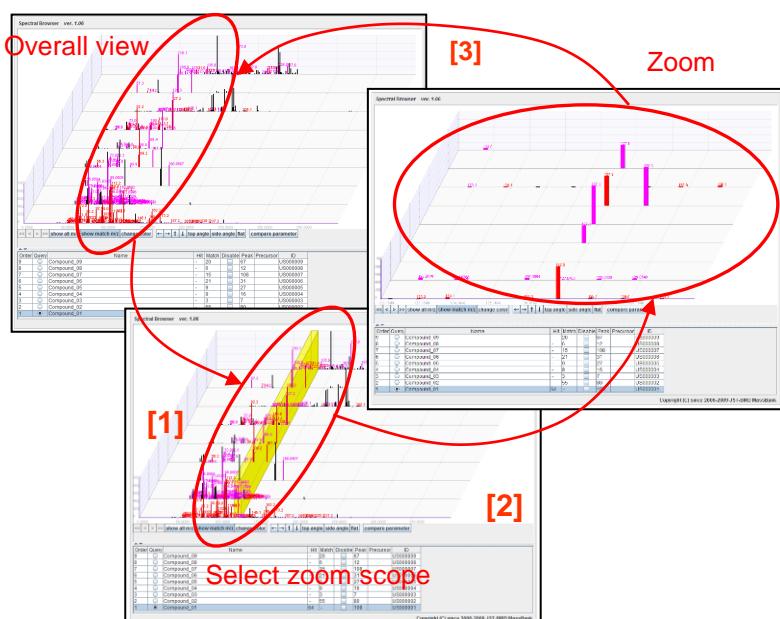


[1] Select query spectrum

Click a radio button for selecting a query. The one-to-many comparison is suddenly executed and its results are reflected automatically.



<<Handy Feature 1: Spectrum Zoom>>



[1] Select location to zoom

Drag from the location of the start of the zoom.

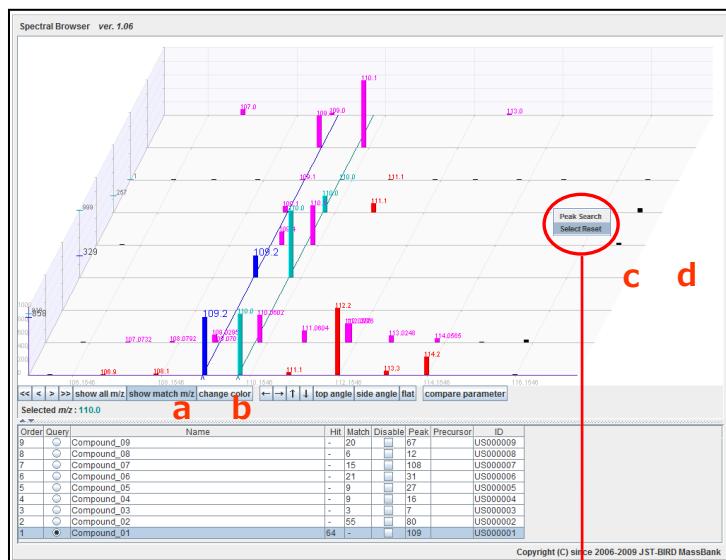
[2] Set zoom position

Drop to set the location on the spectrum to zoom.

[3] End zoom

Double click in comparison window, then return to the initial size without zooming

<< Handy Feature 2: Peak Manipulation>>



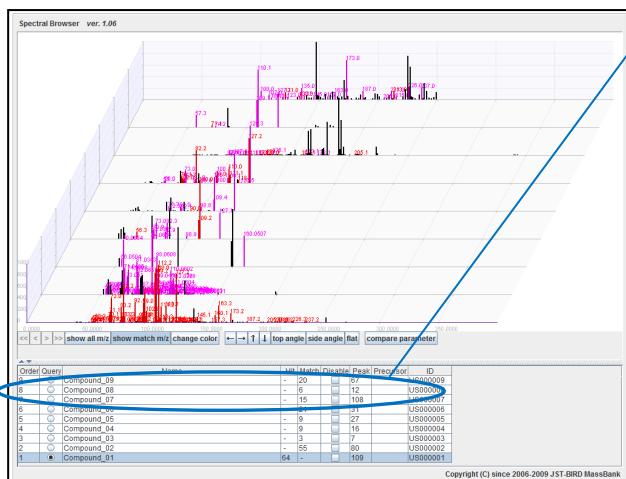
Peak Search Results																																									
mass calculator user manual																																									
Search Quick View Submitter User Account Search Download Help Feedback Logoff																																									
Edit / Recipient Query																																									
Open All Tree Multiple Display Spectrum Search																																									
Results : 2,940 Hits, 1 - 26 Deployed																																									
First 2 3 4 5 6 7 8 9 10 Next Last Total 87 Page																																									
<table border="1"> <thead> <tr> <th></th> <th>Name</th> <th>Count</th> <th>Formula / Structure</th> <th>ExactMass</th> <th>ID</th> </tr> </thead> <tbody> <tr> <td><input checked="" type="checkbox"/></td> <td>(R)-17-METHYL-TESTOSTERONE</td> <td>1 spectrum</td> <td>C20H30O2</td> <td>302.22458</td> <td></td> </tr> <tr> <td><input checked="" type="checkbox"/></td> <td>(+)-ALPHA-CYPERONE</td> <td>1 spectrum</td> <td>C19H22O</td> <td>218.16707</td> <td></td> </tr> <tr> <td><input checked="" type="checkbox"/></td> <td>(+)-ALPHA-IMUROLENE</td> <td>1 spectrum</td> <td>C19H24</td> <td>204.18780</td> <td></td> </tr> <tr> <td><input checked="" type="checkbox"/></td> <td>(+)-CAMPHOR</td> <td>1 spectrum</td> <td>C19H16O</td> <td>189.19912</td> <td></td> </tr> <tr> <td><input checked="" type="checkbox"/></td> <td>(+)-CINCHONINE</td> <td>1 spectrum</td> <td>C19H22N2O</td> <td>294.17321</td> <td>Not Available</td> </tr> </tbody> </table>							Name	Count	Formula / Structure	ExactMass	ID	<input checked="" type="checkbox"/>	(R)-17-METHYL-TESTOSTERONE	1 spectrum	C20H30O2	302.22458		<input checked="" type="checkbox"/>	(+)-ALPHA-CYPERONE	1 spectrum	C19H22O	218.16707		<input checked="" type="checkbox"/>	(+)-ALPHA-IMUROLENE	1 spectrum	C19H24	204.18780		<input checked="" type="checkbox"/>	(+)-CAMPHOR	1 spectrum	C19H16O	189.19912		<input checked="" type="checkbox"/>	(+)-CINCHONINE	1 spectrum	C19H22N2O	294.17321	Not Available
	Name	Count	Formula / Structure	ExactMass	ID																																				
<input checked="" type="checkbox"/>	(R)-17-METHYL-TESTOSTERONE	1 spectrum	C20H30O2	302.22458																																					
<input checked="" type="checkbox"/>	(+)-ALPHA-CYPERONE	1 spectrum	C19H22O	218.16707																																					
<input checked="" type="checkbox"/>	(+)-ALPHA-IMUROLENE	1 spectrum	C19H24	204.18780																																					
<input checked="" type="checkbox"/>	(+)-CAMPHOR	1 spectrum	C19H16O	189.19912																																					
<input checked="" type="checkbox"/>	(+)-CINCHONINE	1 spectrum	C19H22N2O	294.17321	Not Available																																				

Peak Search Results Window

- Highlight & select peak in Spectral Browser -

In Spectral Browser, when you highlight or select a peak in a spectrum, peaks in other spectra are also highlighted or selected if whose m/z are completely equal to the m/z of the highlighted/selected peak.

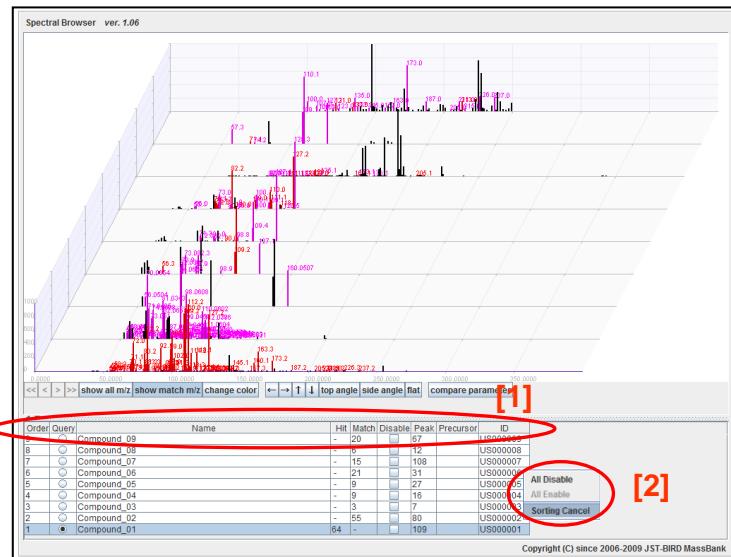
<< Handy Feature 3: Spectrum Manipulation>>



Spectrum Manipulation Buttons

- <<, <, >, >>
 - ... Move display location (only when zoomed on spectrum)
- show all m/z
 - ... Display m/z values of all peaks
- show match m/z
 - ... Display m/z values of matching peaks
- change color
 - ... Change color of entire spectrum
- ←, →, ↑, ↓
 - ... Change angle (manual manipulation)
- top angle
 - ... Change angle (top perspective)
- side angle
 - ... Change angle (side perspective)
- flat
 - ... Change angle (all spectra in flat view)

<< Handy Feature 4: Sort Spectra>>



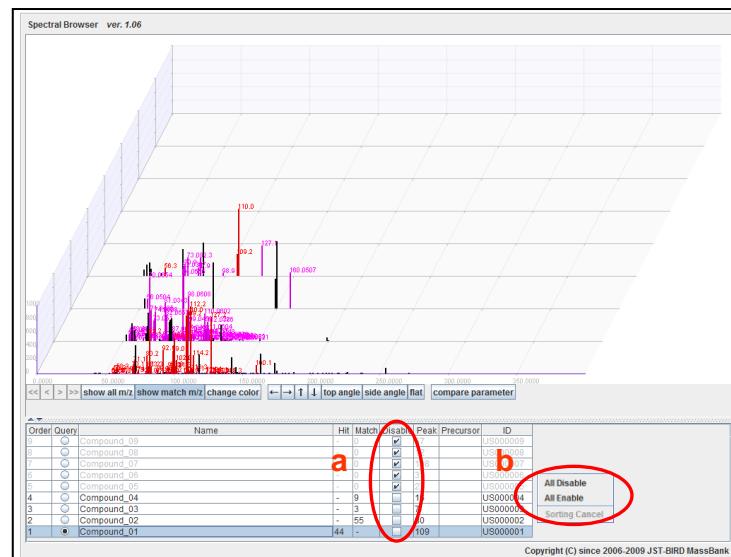
[1] Sort Spectra

Click one of header items in comparison list (i.e. "Order", "Query", "Name", "Hit", "Match", "Disable", "Peak", "Precursor", and "ID"), then the list is sorted by the item. Consecutive clicks of an item change the order of sorting cyclically in ascending, descending and without sorting

[2] Cancel sorting

Select "Sorting Cancel" in a menu popped up by right button click on comparison list.

<< Handy Feature 5: Spectrum Hiding>>



a Hide/show spectrum

For each item in comparison list, tick its checkbox "Disable", then the corresponding spectrum is hided. Untick the checkbox, then it appears again

b Hide/show all spectra

Select "All Disable" in a menu popped up by right button click on comparison list, then all spectra are hided. Select "All Enable" in the same menu, then all spectra appear again.

- Comparison window and comparison list -

Comparison window and Comparison list are operated simultaneously. For example, spectra are sorted in comparison list, the results is suddenly reflected to comparison window and spectra in comparison window are also sorted in same order.

Contact

Please contact the MassBank Group if you have any problems or questions.

massbank@iab.keio.ac.jp

+81-235-29-0800